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**(54) Title:** METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING**(57) Abstract**

The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

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10                   **METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR  
COACTIVATOR BINDING**

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**INTRODUCTION**

20

**Technical Field**

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

**Background**

25                   Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens  
30 (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called "orphan receptors" for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

5 Although overall sequence conservation between nuclear receptors varies between different families of receptors. sequence conservation between functional regions, or modules, of the receptors is high. For example, nuclear receptors can be organized into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-  
10 dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to modulate transcription of DNA, although they may have transcription-independent actions. Nuclear receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear  
15 receptors on transcription. For example, nuclear receptors can stimulate transcription in response to hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al., *Curr. Opin. Cell Biol.* (1997) 9:222-32); and Horwitz et al., *Mol. Endocrinol.* (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain, called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in  
20 coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253; VDR: Jurutka et al., *J. Biol. Chem.* (1997) 272:14592-14599. Masayama et al., *Mol. Endocrinol.* (1997) 11:1507-1517; ER and RAR: Henttu et al., *Mol. Cell Biol.* (1997) 17:1832-1839). While these studies support the physiological relevance of the observed interaction, the structural and functional nature of the site to which coactivators bind has not been defined.

25 The medical importance of nuclear receptors is significant. They have been implicated in breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism, hypercholesterolemia, obesity and other conditions. However, limited treatments are available and current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors  
30 are desired for drug development, the structural and functional basis of such sites, including the coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator proteins. This would provide a major new target for iterative drug design, synthesis, and selection.  
35 It also would be advantageous to devise methods and compositions for reducing the time required to discover compounds that target the coactivator binding site of nuclear receptors and administer them to organisms to modulate physiological processes regulated by nuclear receptors.

5 Relevant Literature

Wagner et al., (*Nature* (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., *supra*; O'Donnell et al., *Mol. Endocrinol.* (1991) 5:94-99; Whitfield et al., *Mol. Endocrinol.* (1995) 9:1166-79; Saatcioglu et al., *Mol. Cell Biol.* (1997) 17:4687-95; Collingwood et al., *supra*; Kamei et al., *Cell* (1996) 85:403-14). Hong et al. (*Proc. Natl. Acad. Sci. USA* (1996) 93(10):498-49452) and Hong et al. (*Mol. Cell. Biol.* (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (*Nature* (1997) 387:677-84), Le Douarin et al., (*EMBO J* (1996) 15:6701-6715) and Heery et al. (*Nature* (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

15

SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by

- 5 binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by  
10 homology to the coactivator binding site of human TR described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

- 15 Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or  
20 in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator  
25 binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a  
30 machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by  
35 modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator

5 binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors. The unique features involved in receptor-selective coactivator binding can be identified by  
10 comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

15

### **BRIEF DESCRIPTION OF THE DRAWINGS**

**Figure 1** shows the specific effects of mutations on hTR $\beta$ 1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T<sub>3</sub> dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant.  
20 GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

**Figure 2** shows that overexpression of full-length GRIP1 rescues loss of transcriptional  
25 activation by hTR $\beta$ 1 mutants. Indicated amounts of the expression vector for full-length GRIP1, pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in **Figure 1**. The WT or different representative hTR $\beta$ 1 mutants are indicated.

**Figure 3** shows specific hER $\alpha$  surface mutants cause loss of transcriptional activation in HeLa cells in parallel with their loss of *in vitro* GRIP1 binding. The fold E<sub>2</sub> activation, expressed as  
30 the percentage of WT, and the phosphorimager quantitation of *in vitro* binding of [<sup>35</sup>S]-labeled hER $\alpha$  WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

5       **Figure 4** shows a plot of the fold  $E_2$  activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for **Figure 3**. The WT or different hER $\alpha$  mutants are indicated. The data represent the averages of three independent experiments, with standard deviations less than 10%.

10       **Figure 5** shows a CPK model of the TR $\alpha$ -LBD, indicating the LBD surface locations of mutations made in the full-length hTR $\beta$ 1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1 $\alpha$  binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues,  
15       respectively. The main chain structures of the TR $\alpha$ - and TR $\beta$ -LBDs are the same (data not shown).

**Figure 6** shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

**Figure 7** shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2,  
20       and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TR $\beta$  LBD. Single letter designations are used for the amino acids.

**Figure 8** shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

25       **Figure 9** shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

**Figure 10** shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of  
30       NR-box-TR $\beta$  LBD interactions.

5       **Figure 11** shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TR $\beta$  LBD.

10       **Figure 12** shows the contents of the asymmetric unit of the crystallized hTR $\beta$  LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in  
15 both bound peptides.

**Figure 13** shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTR $\beta$  LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of  $\alpha$ -helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTR $\beta$  LBD, and the neighboring monomer, are omitted for clarity.

20       **Figure 14** shows interface between the GRIP1 NR-box 2 peptide and the hTR $\beta$  LBD. Side chains of residues of the hTR $\beta$  LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID  
25 NO: 2) ILxxLL motif shown explicitly.

**Figure 15** shows residues in the hTR $\beta$  LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTR $\beta$  LBD.

30       **Figure 16** shows molecular surface of the hTR LBD. The side chains of the leucines residues fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

5           **Figure 17** shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucine residues fit into pockets of the coactivator binding site of the hTR $\beta$  LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

10           **Figure 18** shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding  
15 site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

**Figure 19** shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes  
20 represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.



5

## DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR

5 residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER  
10 LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

15 Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor  
20 structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be  
25 identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor  
30 residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site  
35 may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284, Lys288, Ile302, Lys306, Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus,

5 for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

10 The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and  
15 other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

20 Compounds of particular interest fit spacially and preferentially into the coactivator binding site. By "fits spacially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of  
25 hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a  
30 biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

35 The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single

5 gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR:  $\alpha$ ,  $\beta$ ) or three (RAR, RXR, and PPAR:  $\alpha$ ,  $\beta$ ,  $\gamma$ ) genes or have alternate RNA splicing.

10 The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained  
15 structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface  
20 shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in Figure 19). As described in the Examples, the cocrystal of the hTR $\beta$  LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide.  
25 Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO:  
30 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix  
35 motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

5 For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be used to predict how a small molecule of interest can interact with the nuclear receptor coactivator binding site. Fragment-based docking also can be used in building molecules *de novo* inside the coactivator binding site, by placing chemical fragments that complement the site to optimize  
10 intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new  
15 compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

20 . . . Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule  
25 databases include any virtual or physical database, such as electronic and physical compound library databases. and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR),  
30 using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual  
35 inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and

- 5 molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

- 20 Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, *J. Med. Chem.* (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202; available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, *J. Mol. Biol.* (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

- 30 Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

5 Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., Royal Chem. Soc. (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL  
10 Information Systems, San Leandro, CA; reviewed in Martin, *J. Med. Chem.* (1992) 35:2145-2154); and HOOK (available from Molecular Simulations, Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally  
15 including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

20 Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., *J. Med. Chem.* (1990) 33:883-894); Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of  
25 which may be used. See, for example, Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, *Structure*, (1994) 2:577-587); and Kuntz et al., *Science*, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

30 Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity,  
35 such as a biologically based assay. Screening can be *in vitro* and/or *in vivo*. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening

5 preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

10 As an example, *in vitro* binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160  
15 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein  
20 and in Shibata et al. (*Recent Prog. Horm. Res.* 52:141-164 (1997)); Tagami et al. (*Mol. Cell Biol.* (1997) 17(5):2642-2648); Zhu et al. (*J. Biol. Chem.* (1997) 272(14):9048-9054); Lin et al. (*Mol. Cell Biol.* (1997) 17(10):6131-6138); Kakizawa et al. (*J. Biol. Chem.* (1997) 272(38):23799-23804); and Chang et al. (*Proc. Natl. Acad. Sci. USA* (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments  
25 thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., *MCB supra*; and Hong et al., *PNAS supra*) and/or SRC-1 (Spencer et al., *Nature* (1997) 389:194-198; Onate et al., *Science* (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist  
30 activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric  
35 effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.



5       Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to  
10       measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include  
15       TR-based disorders including cardiovascular disease, metabolic disorders, hyperthyroidism, glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

      The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples,  
20       TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand  $T_3$ .

      Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or  
25       small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

      After the three dimensional structure of the cocrystal is determined, the structural  
30       information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

      Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful  
35       for solving the structure of those other crystal forms of nuclear receptors. They may also be used to

- 5 solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in **Appendix 1**. This method will provide an accurate structural form for the  
10 unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model  
15 of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular  
20 complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interactive drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of  
25 machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of  
30 the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including  
35 members of the steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors

5 that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR- $\alpha$ , human RAR- $\gamma$ , human RXR- $\alpha$ , human RXR- $\alpha$ , human PPAR- $\alpha$ , human PPAR- $\beta$ , human PPAR- $\gamma$ , human VDR, human ER (as described in Seielstad *et al.*, *Molecular Endocrinol.*, (1995) 9:647-658,  
10 incorporated herein by reference), human GR, human PR, human MR, and human AR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2.  
15 A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong *et al.* (*PNAS supra*; and *MCB supra*), for GRIP1 expression, which reference is herein incorporated by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or  
20 as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most  
25 preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR- $\alpha$  or Glu 202 to Asp 461 of the human TR- $\beta$ .

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass  
30 spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC),  
35 and heparin affinity chromatography.

5 To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound  
10 receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with  
15 at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be  
20 established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction  
25 pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can  
30 assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials  
35 at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute

5 components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the hanging drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., supra. The structure is refined following  
10 standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of  
15 the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

5

**EXAMPLES****Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators****A. Human TR $\beta$  LBD**

Human TR $\beta$  LBD (His6-E202-D461) was expressed and purified as described (Shiau et al.,  
10 *Gene* (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28)  
in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for  
24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl,  
10% glycerol, 25mM  $\beta$ -mercaptoethanol and 0.1mM PMSF as described above. The lysate was  
15 cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in  
the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an  
imidazole gradient (12 - 300 mM). TR $\beta$  LBD containing fractions were loaded in 0.6M ammonium  
sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium  
sulfate gradient [0.6 - 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TR $\beta$  LBD  
were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T<sub>3</sub> (Sigma).  
20 The hydrophobic interaction run was repeated with liganded receptor under the same conditions.  
Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed  
to 20mM Hepes pH7.0, 3mM DTT and 0.1 $\mu$ M T<sub>3</sub> using NAP columns (Pharmacia). For  
crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10  
concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter  
25 bacterial culture.

**B. Human TR mutants**

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded  
oligonucleotides which encode the mutant sequence and which have ends allowing them to be  
ligated as a cassette using pairs of the NsiI, PstI, SstI, AlwNI, ApoI, PflMI, BstXI, BseRI, BsmFI,  
30 PvuII, NspI, SmaI, PmlI, BglII and BsmI restriction sites of the hTR $\beta$ 1 cDNA sequence, or the 3'  
plasmid polylinker Sall, or BamHI restriction sites. The hTR $\beta$ 1 sequences thus mutated were  
subcloned into the pCMX vector encoding the full-length 461 amino acid hTR $\beta$ 1 sequence. Some  
of the mutations of the hTR $\beta$ 1 in the CMX vector and all three mutations of the hER $\alpha$  in the pSG5-  
ER-HEGO vector (Tora et al., *EMBO* (1989) 8:1981) were created using Quick Change Site-

- 5 Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

### C. Human ER $\alpha$ LBD

The human ER $\alpha$ -LBD 297-554 was overexpressed as described previously (Seielstad, et al., *supra*) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained  
10 the sequence Met-Asp-Pro fused to residues 297 to 554 of the hER $\alpha$  (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., *Proc. Natl. Acad. Sci. USA* (1980) 77:5115-5119; Landel, et al., *Mol. Endocrinol.* (1994) 8:1407-1419; Landel, et al., *J. Steroid Biochem. Molec. Biol.* (1997) 63:59-73).

15 To carboxymethylate the solvent-accessible cysteines, the bound hER $\alpha$ -LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., *Steroids* (1996) 61:367-373). Protein was eluted with 3 x 10<sup>-5</sup> M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hER $\alpha$ -LBD was typically close to 100% (Seielstad, et al., *Biochemistry* (1995) 34:12605-12615). The affinity-  
20 purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hER $\alpha$ -LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass  
25 spectrometry.

### D. Human ER mutants

To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ER $\alpha$  LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the  
30 binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind <sup>35</sup>S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

5       <sup>35</sup>S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hER $\alpha$  LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376; 10 L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist, 15 confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

#### E. Human ER LBD-GST Fusion Protein

20       A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hER $\alpha$  was constructed by subcloning the EcoRI fragment from pSG5 ER $\alpha$ -LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were 25 created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

#### F. Radiolabeled full-length receptors and coactivator proteins

30       Wild-type (WT) or mutant pCMV-hTR $\beta$ 1 vector and the pSG5-GRIP1 and pCMX-SRC-1a vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the TNT coupled Reticulocyte Lysate System (Promega) and [<sup>35</sup>S]-Met (DuPont). GST-GRIP1 (amino acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-hTR $\beta$ 1 (full-length, WT or mutants, WT provided by C. Costa), and the GST-hRXR $\alpha$  (full-length



- 5 provided by. C. Costa), fusion proteins were produced in *E. coli* strain HB101 as per the manufacturer's protocol (Pharmacia Biotech).

**G. Coactivator GRIP1 563-767 His6 GST fusion protein**

- GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1 563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I-Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freeze-thawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliquots and stored at -70°C.

30 **H. Coactivator GRIP1 563-767 His6**

- GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived from pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. The fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl

- 5 pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

### Example 2: Peptide synthesis

- Coactivator peptides were obtained using standard techniques. All peptides were HPLC  
10 purified and analyzed by mass spectroscopy. Peptide concentrations were either determined spectroscopically using the tyrosine signal ( $A_{276} = 1450 \text{ M}^{-1}\text{cm}^{-1}$ ) or by amino acid analysis following standard techniques.

### Example 3: Binding assays with nuclear receptors and coactivators

#### A. GST-GRIP Pull-down Assays and Peptide Competition Assays

- 15 Binding experiments were performed by mixing glutathione beads containing 10  $\mu\text{g}$  of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2  $\mu\text{l}$  of the [ $^{35}\text{S}$ ]-labeled wild-type or mutant hTR $\beta$ 1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150  $\mu\text{l}$  of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM  $\text{MgCl}_2$ , 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the  
20 presence or absence of 1  $\mu\text{M}$   $\text{T}_3$ . Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

- For *in vitro* binding studies GR, TR and their derivatives were translated in the presence of [ $^{35}\text{S}$ ]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were  
25 performed in the presence and absence of 10 $\mu\text{M}$  dexamethasone or 1 $\mu\text{M}$  RU486 for GR and 10 $\mu\text{M}$  triiodothyronine for TR. Expression was quantified by phosphorimager analysis (BAS2000, Fuji). For all binding assays 50 $\mu\text{l}$  of a 20% bead suspension containing either 1.6 or 4.0  $\mu\text{M}$  bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2 $\mu\text{l}$  or 1.4 $\mu\text{l}$  *in vitro* transcribed and translated TR or GR, respectively. Binding was performed in the binding  
30 buffer described above supplemented with 20  $\mu\text{g}/\text{ml}$  BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of

5 receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200 $\mu$ l binding buffer + BSA at 4°C before elution of the bound proteins in 20 $\mu$ l SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was  
10 determined by phosphoimager analysis.

### B. GST-hTR $\beta$ 1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [ $^{35}$ S]-labeled full-length GRIP1, [ $^{35}$ S]-labeled full-length SRC-1a, and [ $^{35}$ S]-labeled full-length hRXR $\alpha$ , to GST-hTR $\beta$ 1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and  
15 E457K all bound to hRXR $\alpha$  with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [ $^{35}$ S]-Met-labeled full-length hTR $\beta$ 1 WT and mutants (data not shown).

### 20 C. GST-hER $\alpha$ LBD Pull-down Assays

The wild-type and mutant GST-hER $\alpha$  LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hER $\alpha$  (H222). Cleared extracts containing the GST- hER $\alpha$  LBDs were  
25 incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1  $\mu$ M of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10  $\mu$ l glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40.  $^{35}$ S-labeled GRIP1 was synthesized by *in vitro*  
30 transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hER $\alpha$  LBDs were incubated for 2.5 hours with 2.5  $\mu$ l aliquots of crude translation reaction mixture diluted in 300  $\mu$ l of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40,

- 5 proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound  $^{35}\text{S}$ -GRIP1 was quantitated by fluorography following SDS-PAGE.

#### D. Electrophoretic Mobility Shift Assays

- GRIP1, a mouse p160 coactivator, recognizes the ER $\alpha$  LBD in a ligand-dependent manner. The binding of agonists to the ER $\alpha$ LBD promotes recruitment of GRIP1, whereas binding of  
10 antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ER $\alpha$  strongly prefers NR-box 2 (Ding, et al., *Mol. Endocrinol.* (1998) 12:302-13).

- An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ER $\alpha$  LBD in the presence of either DES or OHT. Eight microgram  
15 samples of purified hER $\alpha$ -LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10  $\mu\text{l}$  of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

- 20 In the presence of the NR-box 2 peptide, the migration of the DES-hER $\alpha$ -LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hER $\alpha$ -LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

#### **Example: 4 Transfection assays with TR and hER $\alpha$**

- 25 HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5  $\mu\text{g}$  of the reporter p(DR-4) $_2$ -TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results  
30 (data not shown). Also, 2  $\mu\text{g}$  of the hTR $\beta$ 1 expression vector, pCMX-TR (WT or mutant), and 0.5  $\mu\text{g}$  transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the  $\beta$ -galactosidase gene, were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s),

5 or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., *supra*), and GC cells expressing TR (Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073).

For hER $\alpha$  assays, 5  $\mu$ g of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, *et al.*, *Mol Cell Biol.* (1995) 15:1554), 0.5  $\mu$ g expression vector encoding full-length hER $\alpha$ , pSG5-er HEGO (WT or mutants), and 2  $\mu$ g of 10 p $\beta$ galact, were used. For the experiments of Figures 2 and 4, 0.5  $\mu$ g of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were treated with or without 1  $\mu$ M T<sub>3</sub> or E<sub>2</sub>, as indicated. After culturing for 24 hrs, the LUC or CAT activities were assayed and the  $\beta$ -galactosidase activities were also assayed to correct for 15 differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

#### Example 5: Hormone binding assays for wild-type and mutant TRs

The T<sub>3</sub> binding affinity constants (K<sub>d</sub>) for *in vitro* -translated WT and mutant TRs were measured using [<sup>125</sup>I] 3,5,3'-triiodo-L-thyronine ([<sup>125</sup>I]T<sub>3</sub>) in gel filtration binding assays as 20 described (Apriletti et al., *Protein Expr. Purif.* (1995) 6:363). Both the K<sub>d</sub> and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81  $\pm$  12 pM. The relative affinity was determined by dividing the WT K<sub>d</sub> by each 25 mutant K<sub>d</sub>. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R 30 (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

#### Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3,5,3'-triiodo-L-thyronine (T<sub>3</sub>) bind equally well to the coactivator, GRIP1. In all cases, GRIP1 binding was hormone-dependent

5 (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (**Figure 1**). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (**Figure 1**). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators  
10 recognize the same TR surface residues.

#### **Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell**

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells.  $T_3$  increased reporter gene activity 5-fold in cells  
15 expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in **Figure 1**). By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to  $T_3$  which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of  
20 GRIP1 binding and activation (**Figure 2**). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

#### **Example 8: Effect of TR mutations on other receptor functions**

The effects of the mutations on other receptor functions also were examined. All of the  
25 mutants bound radiolabeled thyroid hormone ( $K_d$  values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region  
30 spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., *supra*; Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of  $T_3$ -dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al., *supra*), suggesting  
35 that the CBS residues do not participate in TR actions mediated through these proteins. These data

- 5 indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

#### Example 9: Coactivator binding site in ER

- 10 Three separate mutations (K362A, V376R, and E542K) were created in human estrogen receptor- $\alpha$  (hER $\alpha$ ) which align to three of the effective positions in hTR $\beta$ 1 (K288A, I302R, and E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which  
15 responds to the ER amino-terminal activation function (Berry et al., *EMBO J* (1990) 9:2811-2818) (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

#### Example 10: Coactivator NR-box binding affinity for TR

- 20 To study the interaction between nuclear receptors and GRIP1 *in vitro*, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using PhD, displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are  
25 part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

- Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTR $\beta$  LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50 ) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine  
30 does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = 1.0  $\mu$ M) over NR-box 3 (EC50 = 4.0  $\mu$ M) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR.

- 5 Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

#### Example 11: Coactivator NR-box binding affinity for GR

GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (Figure 8). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR  
10 about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial antagonist RU486. These results are in agreement with *in vivo* 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the  
15 absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR  
20 prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

#### Example 12: Coactivator peptide binding affinity for TR

To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or  
25 structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTR $\beta$  LBD were performed using coactivator peptides containing different NR-boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLQLDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (Figure 9). Consistent with the interaction of hTR LBD $\beta$  with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of  
30 GRIP1 with hTR $\beta$  LBD only at very high concentrations ( $EC_{50}$  = 130  $\mu$ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTR $\beta$  LBD for NR-box 2 ( $EC_{50}$  (NR-box 2) = 1.5  $\mu$ M,  $EC_{50}$  (NR-box 3) = 4  $\mu$ M). The apparent affinities ( $EC_{50}$ ) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the  
35 sequence and independent of the structural context of the NR-boxes.



5       Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes, TR preferentially binds NR-box 2.

      These results show the preference of TR for NR-box 2 is sequence dependent.

10       The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

### **Example 13: Binding affinity of TR for extended coactivator peptides**

      Sequence identity between all three central NR-boxes of the p160 coactivator family is limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (**Figure 6**). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTR $\beta$  LBD were compared (**Figure 10**).

      A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

      These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adjacent sequences.

## 5 Example 14: Binding affinity of TR and GR for mutant coactivator

### A. TR affinity for ILxxLL motif residues

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRLL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (Figure 11). Surprisingly, replacement of  
10 any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTR $\beta$  LBD, it appears that their contribution to the affinity of NR-box 2 for hTR $\beta$  LBD is cooperative rather than additive.

15 Similar results were obtained by competing the interaction of hTR $\beta$  LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (Figure 11). Whereas the peptides containing the IL or LL replacement failed to interact with the hTR $\beta$  LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal  
20 effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (Figure 11). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues  
25 themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTR $\beta$  LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767)  
30 with hTR $\beta$  LBD.

### B. TR affinity of FxxLW and FxxAL motif residues

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTR $\beta$  LBD:NR-box 2 interaction surface, whereas the non conserved

5 isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTR $\beta$  LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-  
10 KHKILHRLQLDSS-698 is highly complementary to the corresponding binding site in the hTR $\beta$  LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., *Nat Struct Biol.* (1996) 3:87-94; Wagner et al., *supra*; Renaud et al., *Nature* (1995) 378:681-689; Bourguet et al., *Nature* (1995) 375:377-382; and Brzozowski et al., *Nature* (1997) 389:753-758).  
15

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic  $\alpha$ -helices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL)  
20 differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally  
25 interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts  
30 with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very  
35 high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a

- 5 GRIP1 mutant lacking NR-box 3, binds GR *in vivo* (Ding et al., *supra*). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the peptide rather than a particular strong interaction of GR with GRIP1 (563-767).  
10

These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

### C. TR affinity for residues adjacent to ILxxLL motif

- 15 Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (**Figure 11**). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the  
20 original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box  
25 interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.

## **Example 15: Crystallization and Structure Determination of NR LBD Complexes**

### A. Crystallization of hTR $\beta$ LBD with T<sub>3</sub> and GRIP1 NR-box 2 Peptide

- Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the  
30 hTR $\beta$  LBD. The complex of the hTR $\beta$  LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTR $\beta$  LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding

5 of prepared drops with microcrystals of the hTR $\beta$  LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTR $\beta$  LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTR $\beta$  LBD determined previously (Wagner et al., *supra*), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTR $\beta$  LBD, residues K211-P254 and G261-D461 of monomer 2  
10 of the hTR $\beta$  LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-KILHRLLQDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLLQD-696 (Appendix 1).

Briefly, the complex between the hTR $\beta$  LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal)  
15 volumes of a solution of 9mg/ml hTR $\beta$  LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTR $\beta$  LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M  
20 ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10<sup>-3</sup> to 10<sup>-5</sup> dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTR $\beta$  LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6).

5

**Table 1**  
**Data collection, phasing, and refinement statistics**

Data collection						
Data set	Resolution (Å)		Reflections		Coverage (%)	R <sub>sym</sub>
Native	3.6		measured	unique	96.3	0.007
			35565	8490		
Rotation search						
Search model	Euler angles (°)				Correlation coefficient	
		Θ <sub>1</sub>	Θ <sub>2</sub>	Θ <sub>3</sub>	Highest peak	Highest false peak
	hTR β LBD	M1	60.12	80.68	241.90	16.3
	M2	9.93	87.70	180.6	15.9	14.2
Translation search						
		Fractional coordinates			Translation function	
		x	y	z	Highest peak (o)	Highest false peak (o)
	M1	0.522	0.428	0.250	19.52	10.02
	M2	0.200	0.932	0.119	26.11	5.77
Refinement						
	Resolution (Å)		Reflection		R	R <sub>free</sub>
F > 2(	25 - 3.7		7614		0.2990	0.3219
All data	25 - 3.7		7851		0.3010	0.317

$R_{\text{sym}} = \sum_h \sum_i |I_{h,i} - \bar{I}_h| / \sum_h I_h$  for the intensity ( $I$ ) of  $i$  observations of reflection  $h$ .

Correlation coefficient =  $\sum_h E_o^2 E_c^2 - E_o^2 E_c^2 / [\sum_h (E_o^2 - E_o^2)^2 \sum_h (E_c^2 - E_c^2)^2]^{1/2}$

Translation function ( $t_a, t_b, \dots$ ) =  $\sum_h (|E_o(h)|^2 - \sum_h \langle |E_o(h)|^2 \rangle) (E_c(h, t_a, t_b, \dots))^2 - \langle |E_c(h)|^2 \rangle$

where  $E_o$  represents the normalized observed structure factor amplitudes, and  $E_c$  represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation ( $t_a, t_b$ ) of the NCS monomers, divided by the rms value of the translation function density.

R factor =  $\sum |F_{\text{obs}} - F_{\text{calc}}| / \sum |F_{\text{obs}}|$ .

$R_{\text{free}}$  is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

5            **B.     Crystallization of hER $\alpha$  LBD with DES and GRIP1 NR-box 2 Peptide**

Crystals of a DES-hER $\alpha$  LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hER $\alpha$  LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two  $\mu$ L samples of this solution were mixed  
10 with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800  $\mu$ L of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2<sub>1</sub> with cell dimensions a=54.09, b=82.22, c=58.04 and  $\beta$ =111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200  
15  $\mu$ m x 40  $\mu$ m x 40  $\mu$ m crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10  $\mu$ M peptide and frozen in an N<sub>2</sub> stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were  
20 processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *Methods Enzymol.* (1997) 276:307-326) using the default -3 $\sigma$  cutoff.

**C.     Crystallization of hER $\alpha$  LBD with OHT**

Crystals of the hER $\alpha$  LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2  $\mu$ L) of a solution containing 3.9  
25 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800  $\mu$ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6<sub>5</sub>22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit  
30 consists of a single hER $\alpha$  LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400  $\mu$ m x 250  $\mu$ m x 40  $\mu$ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N<sub>2</sub> suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a

- 5 wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *supra*) using the default  $-3\sigma$  cutoff.

**Example 16: Structure determination and refinement of NR LBD complexes**

**A. Structure of hTR $\beta$  LBD with T<sub>3</sub> and GRIP1 NR-box 2 Peptide**

- Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA  
10 with a 0.3mM collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In *Macromolecular Crystallography, Part A* (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in  
15 AMORE from a model of hTR $\beta$  LBD with the ligand, T<sub>3</sub>, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTR $\beta$  LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTR $\beta$  LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and  
20 conventional difference Fourier maps for the iodine atoms of the T<sub>3</sub> ligand confirmed the correctness of the solution. The iodine atoms for both T<sub>3</sub> ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTR $\beta$  LBD. The electron density could be modeled as a short  $\alpha$ -helix, and the observed side chain  
25 density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTR $\beta$  LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTR $\beta$  LBD:GRP1 site 2 peptide complex are attached as  
**Appendix 1.**

30 **B. Structure of hER $\alpha$  LBD with DES and GRIP1 NR-box 2 Peptide**

Initial efforts to determine the structure of the DES-hER $\alpha$  LBD-NR box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4



5 suite: programs for protein crystallography", *Acta Crystallogr.* (1994) D50:760-763) indicated the  
presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by  
molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human  
RAR $\gamma$  LBD (Renaud, et al., *supra*) as the search probe ( $R=58.2\%$ ,  $CC=35.6\%$  after placement of  
10 both monomers). Given that the model at this point was both inaccurate (r.m.s.d.  $1.7 \text{ \AA}$  between  
this model and the final model based on  $C\alpha$  positions) and incomplete (accounting for only  $\sim 45\%$   
of the total scattering matter in the asymmetric unit), an aggressive density modification protocol  
was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with  
model building in MOLOC (Muller, et al., *Bull. Soc. Chim. Belg.* (1988) 97:655-667) and model  
refinement in REFMAC (Murshudov, et al., *Acta Crystallogr.* (1997) D53:240-255) (using tight  
15 NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA  
(Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al,  
eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask  
manipulations and PHASES (Furey, et al., PA33 *Am. Cryst. Assoc. Mtg. Abstr.* (1990) 18:73) and  
the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of  
20 weights.

However, although the DES-hER $\alpha$  LBD-NR complex model accounted for  $\sim 90\%$  of the  
scattering matter in the asymmetric unit, refinement was being hampered by severe model bias.  
The high-resolution data set of the DES-hER $\alpha$  LBD-NR-box 2 peptide complex became available  
when the  $R_{\text{free}}$  of the OHT-hER $\alpha$  LBD model was  $\sim 31\%$ . Both monomers in the asymmetric unit of  
25 the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hER $\alpha$   
LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model.  
The missing parts of the model were built and the rest of the model was corrected using MOLOC  
and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC  
using tight NCS restraints. At later stages, the model was refined without NCS restraints using the  
30 simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximum-  
likelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent  
correction were used. The  $R_{\text{free}}$  set contained a random sample of  $6.5\%$  of all data. In refinement,  
all data between  $27$  and  $2.03 \text{ \AA}$  (with no  $\sigma$  cutoff) were used. The final model was composed of  
residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of  
35 peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride  
ion. According to PROCHECK,  $93.7\%$  of all residues in the model were in the core regions of the  
Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hER $\alpha$

- 5 LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% ( $R_{\text{free}}=25.0\%$ ) using data to 2.03 Å resolution.

Ile 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The  $\gamma$ -carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 10 377, the  $\gamma$ -carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ER $\alpha$  LBD (Eng, et al., *Mol. Cell. Biol.* (1997) 17:4644-4653); Lazennec, et al., *Mol. Endocrinol.* (1997) 11:1375-86; White, et al., *EMBO J.* (1997) 16:1427-35). Atomic coordinates of 15 DES-LBD-peptide complex are attached as **Appendix 2**.

5

Table 2

## Summary of Crystallographic Statistics

	<u>Data Collection</u>	<u>Ligand</u>	
		<u>DES</u>	<u>OHT</u>
10	Space group	P2 <sub>1</sub>	P6 <sub>5</sub> 22
	Resolution	2.03	1.90
	Observations	104189	269253
	Unique	30265	23064
	Completeness (%)	98.4	99.1
	R <sub>sym</sub> (%) <sup>a</sup>	7.8	7.0
15	Average I/σI	9.8	16.1
	<u>Refinement</u>		
	Number of non-hydrogen atoms	4180	2070
20	R <sub>cryst</sub> (%) <sup>b</sup> /R <sub>free</sub> (%)	19.9/25.0	23.0/26.1
	Bond r.m.s. deviation (Å)	0.006	0.006
	Angle r.m.s. deviation (°)	1.05	1.05
	Average B factor (Å <sup>2</sup> )	34.0	40.4
	<sup>a</sup> R <sub>sym</sub> = $\sum_i  I_i - \langle I_i \rangle  / \sum_i I_i$ where $\langle I_i \rangle$ is the average intensity over symmetry equivalents		
25	<sup>b</sup> R <sub>cryst</sub> = $\sum  F_o - F_c  / \sum  F_o $		

C. Structure of hERα LBD-OHT complex

30 The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERα LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6<sub>1</sub>22 and P6<sub>5</sub>22. A translation search in P6<sub>5</sub>22 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hERα LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR

5 (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., *Proc. Natl. Acad. Sci. USA* (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the  $R_{\text{free}}$  set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no  $\sigma$  cutoff) were included. The final model consisted of residues 306-10 551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hER $\alpha$  LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% ( $R_{\text{free}}$ =26.2%). Atomic coordinates of OHT-hER $\alpha$  LBD complex are attached as **Appendix 3**.

## 15 **Example 17: Structural analysis of hTR $\beta$ LBD:GRIP 1 NR-box 2 peptide complex**

### **A. Structure of cocrystal complex (contents of asu)**

The asymmetric unit (asu) of the crystal contains two monomers of the hTR $\beta$  LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (**Figure 12**). The structure of the hTR $\beta$  LBD, which closely resembles that of the rTR $\alpha$  LBD (Wagner et al., *supra*), consists of twelve alpha-helices and two  $\beta$ -strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTR $\beta$  LBD and the rTR $\alpha$  LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic  $\alpha$ -helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

25 The relation of the two monomers of the hTR $\beta$  LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., *supra*; Brzozowski et al., *supra*). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the alpha-helix of the cocrystal peptide contacts monomer 1 of the hTR $\beta$  LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

5       The common interface between both cocrystal peptides and the hTR $\beta$  LBD buries the hydrophobic residues that define the cocrystal peptide (SEQ ID NO: 1) LxxLL sequence motif, residues Ile689, Leu690, Leu693, and Leu694; against the surface of the receptor LBD (Figures 16 and 17). The presence of the second peptide in the crystal, duplicating the interactions of the hydrophobic residues, suggests those interactions are specific and drive the interaction of the peptide with the hTR $\beta$  LBD, while the hydrophilic interactions provide a fortuitous crystal contact and account for the dependence of crystallization on the presence and concentration of the peptide.

#### B.     Structure of the GRIP1 NR-box 2 peptide

15       The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLQLDSS-698). For the NR-box 2 peptide in monomer 1 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., *Science* (1996) 274:948-953), VP16:TAF31 (Uesugi et al., *Science* (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan et al., *Cell* (1997) 91:741-752).

#### C.     Structure of the hTR $\beta$ LBD:GRIP1 NR-box 2 peptide interface

30       The hTR $\beta$  LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are I280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

      The GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but

5 defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue  
10 L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTRB LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

### Example 18: Overall Structure of the DES-hER $\alpha$ -LBD-NR-box 2 Peptide Complex

15 The asymmetric unit of the DES-hER $\alpha$  LBD-NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E<sub>2</sub> and RAL (Brzozowski, et al., *supra* and Tanenbaum, et al., *supra*). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar  
20 structures (r.m.s.d. 0.47 Å based on C $\alpha$  positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E<sub>2</sub> (Brzozowski, et al., *supra*); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic  
25 cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic  $\alpha$  helix.  
30 Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

### Example 19: Structure of the OHT-hER $\alpha$ LBD Complex

The binding of OHT induces a conformation of the hER $\alpha$  LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES

5 complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket  
10 as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., *supra*).

#### Example 20: Coactivator binding site structure and function

##### 15 A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the  
20 design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., **Figures 5, 14, and 15**). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that  
25 NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453,  
30 L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational  
35 change upon hormone binding included Leu454 and Glu457. Thus, the site identified by

5 mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site  
 10 are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19).

The coactivator binding site of TR contains charged and hydrophobic residues at its  
 15 periphery, but only hydrophobic residues at its center (see, e.g., Figures 5 and 18). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (Figure 18), right). Residues contained in helices 3, 5 and 6 (Figure 18, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of  
 20 the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (Figure 18, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in  
 25 the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

### B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER $\alpha$  LBD buries 1000 Å<sup>2</sup> of predominantly hydrophobic surface area from both  
 30 molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization  
 35 of the binding site of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER $\alpha$  LBD, which is the same NR-box 2 peptide utilized to crystallize the T<sub>3</sub>-TR



5 LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear  
receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter.  
These residues are highly conserved among the nuclear receptor super family (Figure 19).  
Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of  
exploiting the slight differences among the coactivator binding sites of nuclear receptors in  
10 designing and identifying compounds that target specific nuclear receptors.

The ER $\alpha$  LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-  
KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6)  $\alpha$  helix formed by the side chains of  
Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The  
side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with  
15 the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is  
similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile  
358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689  
and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile  
689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The  
20 side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix  
project away from the ER $\alpha$  receptor and either interact predominantly with solvent or form  
symmetry contacts. None of the side chains of the polar and charged residues outside the helical  
region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is  
25 involved in hydrogen bonds or salt bridges with its associated ER $\alpha$  LBD monomer. The  $\epsilon$ -amino  
group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of  
monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-  
terminal three residues of peptide B are displaced from monomer B and interact extensively with a  
symmetry-related ER $\alpha$  LBD.

30 In addition to interacting with the hydrophobic face of the peptide helix, the ER $\alpha$  LBD  
stabilizes the main chain conformation of the NR box peptide by forming capping interactions with  
both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide  
binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain  
and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These  
35 interactions position the stabilizing charges of the  $\gamma$ -carboxylate of Glu 542 and  $\epsilon$ -amino group of  
Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542

5 hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the  $\epsilon$ -amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

10 Except for the orientation of helix 12, the structure of the peptide binding groove of the ER $\alpha$  LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

15 Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) LLEML instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove  
20 and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions.  
25 Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its  $\epsilon$ -amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu  
30 380. The Glu 380  $\gamma$ -carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER $\alpha$  LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van  
35 der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the

- 5 OHT complex buries more solvent accessible surface area ( $\sim 1200 \text{ \AA}^2$ ) than the NR box peptide in the DES-ER $\alpha$  LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator proteins to nuclear receptors for all members of the nuclear receptor super family.

### REFERENCES

1. U.S. Patent No. 5,331,573
2. U.S. Patent No. 5,500,807
- 20 3. Adams, P. D., Pannu, N. S., Read, R. J., and Brunger, A. T. (1997). *Proc. Natl. Acad. Sci. USA* 94, 5018-23.
4. Apriletti et al., *Protein Expr. Purif.* (1995) 6:363
5. Bartlett et al., In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196
- 25 6. Berry, M., Metzger, D., and Chambon, P. (1990). *EMBO J* 9, 2811-8.
7. Bohm, J. *Comp. Aid. Molec. Design* (1992) 6:61-78
8. Bourguet, W., Ruff, M., Chambon, P., Gronemeyer, H., and Moras, D. (1995). *Nature* 375, 377-82.
9. Brzozowski, A., Pike, A., Dauter, Z., Hubbard, R., Bonn, T., Engstrom, O., Ohman, L., Greene, G., Gustafsson, J., and Carlquist, M. (1997). *Nature* 389, 753-758.
- 30 10. Chang et al., *Proc. Natl. Acad. Sci. USA* (1997) 94(17):9040-9045
11. Cohen et al., *J. Med. Chem.* (1990) 33:883-894
12. Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253
13. DesJalais et al., *J. Med. Chem.* (1988) 31:722-729

- 5 14. Ding, S., Anderson, C., Ma, H., Hong, H., Uht, R., Kushner, P., and Stallcup, M. (1998). *Mol. Endocrinol.* 12, 302-313.
15. Eng, F. C. S., Lee, H. S., Ferrara, J., Willson, T. M., and White, J. H. (1997). *Mol. Cell. Biol.* 17, 4644-4653.
16. Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980)
- 10 17. Furey, et al., PA33 *Am. Cryst. Assoc. Mtg. Abstr.* (1990) 18:73
18. Glass, C. K., Rose, D. W., and Rosenfeld, M. G. (1997). Nuclear receptor coactivators. *Curr. Opin. Cell Biol.* 9, 222-32.
19. Goodford, *J. Med. Chem.* (1985) 28:849-857
20. Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202
- 15 21. Greene, G., Harris, K., Bova, R., Kinders, R., Moore, B., and Nolan, C. (1988). *Mol. Endocrinol.* 2, 714-726.
22. Greene, G., Nolan, C., Engler, J., and Jensen, E. (1980). *Proc. Natl. Acad. Sci. USA* 77, 5115-5119.
23. Heery, D., Kalkhoven, E., Hoare, S., and Parker, M. (1997). *Nature* 387, 733-736.
- 20 24. Hegy, G., Shackleton, C., Carlquist, M., Bonn, T., Engstrom, O., Sjöholm, P., and Witkowska, H. (1996). *Steroids* 61, 367-373.
25. Henttu, P. M., Kalkhoven, E., and Parker, M. G. (1997). *Mol. Cell. Biol.* 17, 1832-9.
26. Hong et al., *Mol. Cell Biol.* (1997) 17:2735-44
27. Hong, H., Kohli, K., Trivedi, A., Johnson, D. L., and Stallcup, M. R. (1996). *Proc. Natl. Acad. Sci. USA* 93, 4948-4952.
28. Horwitz et al., *Mol. Endocrinol.* (1996) 10:1167-77
29. Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976
30. Jurutka et al., *J. Biol. Chem.* (1997) 272:14592-14599
31. Kakizawa et al., *J. Biol. Chem.* (1997) 272(38):23799-23804
- 30 32. Kamei, Y., Xu, L., Heinzl, T., Torchia, J., Kurokawa, R., Gloss, B., Lin, S. C., Heyman, R. A., Rose, D. W., Glass, C. K., and Rosenfeld, M. G. (1996). *Cell* 85, 403-14.
33. Kuiper, G. G., Carlsson, B., Grandien, K., Enmark, E., Haggblad, J., Nilsson, S., and Gustafsson, J. A. (1997). *Endocrinology* 138, 863-70.
34. Kuntz et al, *J. Mol. Biol.* (1982) 161:269-288
- 35 35. Kuntz et al., *Science*, (1992) 257:1078-1082
36. Kussie et al., *Science* (1996) 274:948-953

- 5 37. Landel, C., Kushner, P., and Greene, G. (1994). *Mol. Endocrinol.* 8, 1407-1419.
38. Landel, C., Potthoff, S., Nardulli, A., Kushner, J., and Greene, G. (1997). *J. Steroid Biochem. Molec. Biol.* 63, 59-73.
39. Lazennec, G., Ediger, T. R., Petz, L. N., Nardulli, A. M., and Katzenellenbogen, B. S. (1997). *Mol. Endocrinol.* 11, 1375-86.
- 10 40. Le Douarin, B., Nielsen, A. L., Garnier, J. M., Ichinose, H., Jeanmougin, F., Losson, R., and Chambon, P. (1996). *EMBO J* 15, 6701-15.
41. Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873
42. Lin et al., *Mol. Cell Biol.* (1997) 17(10):6131-6138
43. Masayama et al., *Mol. Endocrinol.* (1997) 11:1507-1517
- 15 44. Meng et al., *J. Comp. Chem.* (1992) 13:505-524
45. Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34
46. Muller, K., Amman, H. J., Doran, D. M., Gerber, P. R., Gubernator, K., and Schrepfer, G. (1988). *Bull. Soc. Chim. Belg.* 97, 655-667.
47. Murshudov, G. N., Vagin, A. A., and Dodson, E. J. (1997). *Acta Crystallogr. D* 53, 240-255.
- 20 48. Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210
49. Nishibata et al., *Tetrahedron* (1991) 47:8985;
50. Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073
51. Norris, J. D., Fan, D., Stallcup, M. R., and McDonnell, D. P. (1998). *J Biol Chem* 273, 6679-88.
52. O'Donnell et al., *Mol. Endocrinol.* (1991) 5:94-99
- 25 53. Onate et al., *Science* (1995) 270:1354-1357
54. Radhakrishnan et al., *Cell* (1997) 91:741-752
55. Renaud, J., Rochel, N., Ruff, M., Vivat, V., Chambon, P., Gronemeyer, H., and Moras, D. (1995). *Nature* 378, 681-689.
56. Saatcioglu et al., *Mol. Cell Biol.* (1997) 17:4687-4695
- 30 57. Sadovsky, et al., *Mol Cell Biol.* (1995) 15:1554
58. Seielstad, D., Carlson, K., Katzenellenbogen, J., Kushner, P., and Greene, G. (1995a). *Mol. Endocrinol.* 9, 647-658.
59. Seielstad, et al., *Biochemistry* (1995) 34:12605-12615
60. Shiau et al. *Gene* (1996) 179(2):205-10

- 5 61. Shibata et al., *Recent Prog. Horm. Res.* 52:141-164 (1997)
62. Spencer, T. E., Jenster, G., Burcin, M. M., Allis, C. D., Zhou, J., Mizzen, C. A., McKenna, N. J., Onate, S. A., Tsai, S. Y., Tsai, M. J., and O'Malley, B. W. (1997). *Nature* 389, 194-8.
63. Tagami et al., *Mol. Cell Biol.* (1997) 17(5):2642-2648
- 10 64. Tanenbaum, D. M., Wang, Y., Williams, S. P., and Sigler, P. B. (1998). *Proc. Natl. Acad. Sci. U S A* 95, 5998-6003.
65. Tora, L., Mullick, A., Metzger, D., Ponglikitmongkol, M., Park, I., and Chambon, P. (1989). *EMBO J* 8, 1981-6.
66. Torchia, J., Rose, D., Inostroza, J., Kamel, Y., Westin, S., Glass, C., and Rosenfeld, M. (1997). *Nature* 387, 677-684.
- 15 67. Uesugi et al., *Science* (1996) 277:1310-1313
68. Verlinde, *Structure*, (1994) 2:577-587
69. Wagner, R., Apriletti, J., McGrath, M., West, B., Baxter, J., and Fletterick, R. (1995). *Nature* 378, 690-697.
70. Webb et al., *Mol Endocrinol* (1995) 9:443
- 20 71. White, R., Sjoberg, M., Kalkhoven, E., and Parker, M. G. (1997). *EMBO J* 16, 1427-35.
72. Whitfield et al., *Mol. Endocrinol.* (1995) 9:1166-79
73. Wurtz, J. M., Bourguet, W., Renaud, J. P., Vivat, V., Chambon, P., Moras, D., and Gronemeyer, H. (1996). *Nat. Struct. Biol.* 3, 87-94.
74. Zhu et al., *J. Biol. Chem.* (1997) 272(14):9048-9054

25

All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

30 The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

## Appendix 1

```

REMARK full length numbering
10  REMARK all residue names correct
    REMARK peptide sequence
    REMARK two molecules of TRB - CHAIN A and CHAIN B
    REMARK two molecules of T3 - CHAIN J and CHAIN K
    REMARK two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y
15  REMARK chain X lies between A and B
    REMARK chain Y interacts with B only
    REMARK residues differing between A and B include:
    REMARK A 217 Glu, A 252 Gln, A 263 Lys (missing side chains)
    REMARK B 237 Ser, B239 His, B 394 Lys (missing side chains)
20  REMARK additionally Gly 261, Gly 262 are not visible in chain A
    REMARK residues differing between X and Y include:
    REMARK A 692 Arg
    REMARK additionally, residues Lys 688, Lys 689; Ser 697, Ser 698
    REMARK are not visible in chain Y

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BNSDOCID: <WO\_\_\_\_\_9960014A2 | >

5	ATOM	35	O	THR	A	215	41.816	17.501	44.691	1.00	53.48	8
	ATOM	36	N	ASP	A	216	43.118	15.683	44.607	1.00	58.81	7
	ATOM	37	CA	ASP	A	216	41.973	14.740	44.615	1.00	61.51	6
	ATOM	38	CB	ASP	A	216	42.386	13.451	45.343	1.00	70.57	6
	ATOM	39	CG	ASP	A	216	42.399	12.283	44.475	1.00	78.07	6
10	ATOM	40	OD1	ASP	A	216	41.532	12.161	43.586	1.00	82.31	8
	ATOM	41	OD2	ASP	A	216	43.293	11.436	44.684	1.00	86.55	8
	ATOM	42	C	ASP	A	216	40.640	15.311	45.268	1.00	58.42	6
	ATOM	43	O	ASP	A	216	39.598	14.840	44.924	1.00	56.85	8
	ATOM	44	N	GLU	A	217	40.673	16.270	46.217	1.00	54.92	7
15	ATOM	45	CA	GLU	A	217	39.502	16.937	46.856	1.00	53.37	6
	ATOM	46	CB	GLU	A	217	39.943	17.459	48.216	1.00	51.02	6
	ATOM	47	C	GLU	A	217	39.113	18.144	45.956	1.00	53.55	6
	ATOM	48	O	GLU	A	217	37.905	18.394	45.695	1.00	54.33	8
	ATOM	49	N	GLU	A	218	40.162	18.895	45.511	1.00	49.20	7
20	ATOM	50	CA	GLU	A	218	39.933	20.073	44.661	1.00	45.94	6
	ATOM	51	CB	GLU	A	218	41.232	20.855	44.304	1.00	43.43	6
	ATOM	52	CG	GLU	A	218	41.907	21.579	45.479	1.00	40.86	6
	ATOM	53	CD	GLU	A	218	43.061	22.446	45.074	1.00	39.88	6
	ATOM	54	OE1	GLU	A	218	43.895	22.019	44.232	1.00	37.61	8
25	ATOM	55	OE2	GLU	A	218	43.183	23.583	45.599	1.00	34.01	8
	ATOM	56	C	GLU	A	218	39.249	19.647	43.390	1.00	44.71	6
	ATOM	57	O	GLU	A	218	38.302	20.291	42.964	1.00	45.31	8
	ATOM	58	N	TRP	A	219	39.720	18.553	42.797	1.00	44.02	7
	ATOM	59	CA	TRP	A	219	39.109	18.061	41.574	1.00	46.97	6
30	ATOM	60	CB	TRP	A	219	39.799	16.793	41.074	1.00	48.42	6
	ATOM	61	CG	TRP	A	219	40.879	17.029	40.141	1.00	54.61	6
	ATOM	62	CD2	TRP	A	219	40.755	17.256	38.733	1.00	55.24	6
	ATOM	63	CE2	TRP	A	219	42.067	17.523	38.245	1.00	53.67	6
	ATOM	64	CE3	TRP	A	219	39.691	17.234	37.828	1.00	54.55	6
35	ATOM	65	CD1	TRP	A	219	42.159	17.159	40.447	1.00	55.75	6
	ATOM	66	NE1	TRP	A	219	42.895	17.485	39.339	1.00	54.43	7
	ATOM	67	CZ2	TRP	A	219	42.330	17.851	36.895	1.00	52.54	6
	ATOM	68	CZ3	TRP	A	219	39.943	17.535	36.509	1.00	55.17	6
	ATOM	69	CH2	TRP	A	219	41.239	17.820	36.029	1.00	55.59	6
40	ATOM	70	C	TRP	A	219	37.646	17.743	41.812	1.00	47.32	6
	ATOM	71	O	TRP	A	219	36.788	18.028	40.978	1.00	43.56	8
	ATOM	72	N	GLU	A	220	37.376	17.142	42.965	1.00	49.91	7
	ATOM	73	CA	GLU	A	220	36.021	16.769	43.316	1.00	53.57	6
	ATOM	74	CB	GLU	A	220	36.052	16.055	44.649	1.00	58.18	6
45	ATOM	75	CG	GLU	A	220	35.149	14.930	44.672	1.00	73.13	6
	ATOM	76	CD	GLU	A	220	35.735	13.935	45.442	1.00	80.06	6
	ATOM	77	OE1	GLU	A	220	36.886	13.575	45.173	1.00	82.12	8
	ATOM	78	OE2	GLU	A	220	35.078	13.478	46.378	1.00	82.78	8
	ATOM	79	C	GLU	A	220	35.161	18.026	43.381	1.00	50.51	6
50	ATOM	80	O	GLU	A	220	33.991	18.010	42.995	1.00	49.94	8
	ATOM	81	N	LEU	A	221	35.761	19.120	43.865	1.00	43.71	7
	ATOM	82	CA	LEU	A	221	35.047	20.398	43.951	1.00	42.81	6
	ATOM	83	CB	LEU	A	221	35.935	21.510	44.510	1.00	39.21	6
	ATOM	84	CG	LEU	A	221	35.375	22.908	44.353	1.00	36.34	6
55	ATOM	85	CD1	LEU	A	221	33.941	22.929	44.836	1.00	36.93	6
	ATOM	86	CD2	LEU	A	221	36.226	23.910	45.122	1.00	24.18	6
	ATOM	87	C	LEU	A	221	34.563	20.815	42.575	1.00	43.46	6
	ATOM	88	O	LEU	A	221	33.392	21.104	42.395	1.00	45.25	8



5	ATOM	89	N	ILE	A	222	35.498	20.871	41.628	1.00	39.09	7
	ATOM	90	CA	ILE	A	222	35.192	21.226	40.254	1.00	35.47	6
	ATOM	91	CB	ILE	A	222	36.379	20.997	39.343	1.00	33.74	6
	ATOM	92	CG2	ILE	A	222	35.970	21.182	37.893	1.00	28.86	6
	ATOM	93	CG1	ILE	A	222	37.532	21.922	39.707	1.00	33.33	6
10	ATOM	94	CD1	ILE	A	222	38.804	21.586	39.004	1.00	34.85	6
	ATOM	95	C	ILE	A	222	34.067	20.365	39.735	1.00	34.26	6
	ATOM	96	O	ILE	A	222	33.033	20.873	39.319	1.00	31.90	8
	ATOM	97	N	LYS	A	223	34.301	19.058	39.750	1.00	39.49	7
	ATOM	98	CA	LYS	A	223	33.316	18.100	39.276	1.00	44.43	6
15	ATOM	99	CB	LYS	A	223	33.603	16.713	39.852	1.00	50.81	6
	ATOM	100	CG	LYS	A	223	32.741	15.631	39.227	1.00	62.51	6
	ATOM	101	CD	LYS	A	223	32.859	14.291	39.943	1.00	72.22	6
	ATOM	102	CE	LYS	A	223	31.798	13.318	39.430	1.00	74.55	6
	ATOM	103	NZ	LYS	A	223	31.900	11.985	40.106	1.00	75.78	7
20	ATOM	104	C	LYS	A	223	31.913	18.565	39.681	1.00	42.81	6
	ATOM	105	O	LYS	A	223	30.936	18.323	38.984	1.00	40.36	8
	ATOM	106	N	THR	A	224	31.849	19.236	40.833	1.00	39.89	7
	ATOM	107	CA	THR	A	224	30.602	19.792	41.378	1.00	39.93	6
	ATOM	108	CB	THR	A	224	30.805	20.206	42.851	1.00	40.57	6
25	ATOM	109	OG1	THR	A	224	31.330	19.113	43.616	1.00	39.27	8
	ATOM	110	CG2	THR	A	224	29.500	20.684	43.461	1.00	38.11	6
	ATOM	111	C	THR	A	224	30.167	21.011	40.533	1.00	39.96	6
	ATOM	112	O	THR	A	224	29.313	20.899	39.655	1.00	36.67	8
	ATOM	113	N	VAL	A	225	30.777	22.160	40.832	1.00	38.02	7
30	ATOM	114	CA	VAL	A	225	30.532	23.426	40.137	1.00	38.12	6
	ATOM	115	CB	VAL	A	225	31.797	24.292	40.122	1.00	38.19	6
	ATOM	116	CG1	VAL	A	225	31.512	25.636	39.491	1.00	36.77	6
	ATOM	117	CG2	VAL	A	225	32.343	24.464	41.505	1.00	41.76	6
	ATOM	118	C	VAL	A	225	30.070	23.195	38.706	1.00	37.52	6
35	ATOM	119	O	VAL	A	225	29.119	23.803	38.239	1.00	36.77	8
	ATOM	120	N	THR	A	226	30.783	22.316	38.018	1.00	34.02	7
	ATOM	121	CA	THR	A	226	30.489	21.971	36.636	1.00	34.67	6
	ATOM	122	CB	THR	A	226	31.565	20.999	36.083	1.00	30.56	6
	ATOM	123	OG1	THR	A	226	32.805	21.696	35.889	1.00	32.20	8
40	ATOM	124	CG2	THR	A	226	31.108	20.346	34.783	1.00	20.99	6
	ATOM	125	C	THR	A	226	29.100	21.361	36.510	1.00	36.41	6
	ATOM	126	O	THR	A	226	28.255	21.877	35.785	1.00	39.64	8
	ATOM	127	N	ALA	A	227	28.880	20.260	37.222	1.00	39.20	7
	ATOM	128	CA	ALA	A	227	27.602	19.562	37.204	1.00	36.93	6
45	ATOM	129	CB	ALA	A	227	27.526	18.600	38.381	1.00	38.06	6
	ATOM	130	C	ALA	A	227	26.507	20.604	37.318	1.00	37.69	6
	ATOM	131	O	ALA	A	227	25.444	20.489	36.718	1.00	40.94	8
	ATOM	132	N	ALA	A	228	26.811	21.630	38.107	1.00	32.86	7
	ATOM	133	CA	ALA	A	228	25.903	22.734	38.356	1.00	32.48	6
50	ATOM	134	CB	ALA	A	228	26.448	23.587	39.486	1.00	28.25	6
	ATOM	135	C	ALA	A	228	25.732	23.570	37.101	1.00	36.12	6
	ATOM	136	O	ALA	A	228	24.673	23.560	36.473	1.00	37.86	8
	ATOM	137	N	HIS	A	229	26.782	24.306	36.752	1.00	33.58	7
	ATOM	138	CA	HIS	A	229	26.762	25.158	35.585	1.00	32.97	6
55	ATOM	139	CB	HIS	A	229	28.155	25.691	35.266	1.00	33.69	6
	ATOM	140	CG	HIS	A	229	28.250	26.333	33.929	1.00	28.39	6
	ATOM	141	CD2	HIS	A	229	29.025	26.081	32.838	1.00	28.83	6
	ATOM	142	ND1	HIS	A	229	27.386	27.368	33.542	1.00	30.47	7

5	ATOM	143	CE1	HIS	A	229	27.654	27.692	32.280	1.00	26.95	6
	ATOM	144	NE2	HIS	A	229	28.635	26.934	31.840	1.00	31.27	7
	ATOM	145	C	HIS	A	229	26.225	24.541	34.312	1.00	38.40	6
	ATOM	146	O	HIS	A	229	25.591	25.227	33.528	1.00	41.49	8
	ATOM	147	N	VAL	A	230	26.519	23.256	34.113	1.00	38.55	7
10	ATOM	148	CA	VAL	A	230	26.088	22.554	32.916	1.00	40.40	6
	ATOM	149	CB	VAL	A	230	26.890	21.256	32.701	1.00	44.68	6
	ATOM	150	CG1	VAL	A	230	26.557	20.656	31.345	1.00	39.39	6
	ATOM	151	CG2	VAL	A	230	28.381	21.509	32.817	1.00	42.18	6
	ATOM	152	C	VAL	A	230	24.603	22.239	32.900	1.00	44.28	6
15	ATOM	153	O	VAL	A	230	23.959	22.316	31.847	1.00	45.94	8
	ATOM	154	N	ALA	A	231	24.072	21.862	34.059	1.00	45.59	7
	ATOM	155	CA	ALA	A	231	22.669	21.500	34.175	1.00	47.84	6
	ATOM	156	CB	ALA	A	231	22.482	20.582	35.374	1.00	45.08	6
	ATOM	157	C	ALA	A	231	21.792	22.734	34.314	1.00	48.04	6
20	ATOM	158	O	ALA	A	231	20.565	22.647	34.324	1.00	49.95	8
	ATOM	159	N	THR	A	232	22.436	23.894	34.384	1.00	47.26	7
	ATOM	160	CA	THR	A	232	21.722	25.161	34.528	1.00	43.64	6
	ATOM	161	CB	THR	A	232	22.112	25.832	35.850	1.00	41.93	6
	ATOM	162	OG1	THR	A	232	23.467	26.283	35.791	1.00	39.10	8
25	ATOM	163	CG2	THR	A	232	21.990	24.846	37.008	1.00	29.80	6
	ATOM	164	C	THR	A	232	22.055	26.114	33.387	1.00	43.97	6
	ATOM	165	O	THR	A	232	21.679	27.279	33.436	1.00	40.55	8
	ATOM	166	N	ASN	A	233	22.783	25.625	32.381	1.00	48.62	7
	ATOM	167	CA	ASN	A	233	23.134	26.468	31.231	1.00	58.62	6
30	ATOM	168	CB	ASN	A	233	24.626	26.283	30.880	1.00	62.44	6
	ATOM	169	CG	ASN	A	233	25.141	27.355	29.927	1.00	68.35	6
	ATOM	170	OD1	ASN	A	233	24.822	28.544	30.096	1.00	65.50	8
	ATOM	171	ND2	ASN	A	233	25.951	26.951	28.959	1.00	74.29	7
	ATOM	172	C	ASN	A	233	22.241	26.035	30.073	1.00	65.06	6
35	ATOM	173	O	ASN	A	233	22.312	24.900	29.604	1.00	69.47	8
	ATOM	174	N	ALA	A	234	21.381	26.954	29.646	1.00	68.80	7
	ATOM	175	CA	ALA	A	234	20.423	26.708	28.564	1.00	70.98	6
	ATOM	176	CB	ALA	A	234	19.748	28.015	28.186	1.00	71.43	6
	ATOM	177	C	ALA	A	234	20.988	26.062	27.308	1.00	73.83	6
40	ATOM	178	O	ALA	A	234	22.041	26.419	26.822	1.00	74.33	8
	ATOM	179	N	GLN	A	235	20.227	25.096	26.819	1.00	75.07	7
	ATOM	180	CA	GLN	A	235	20.562	24.363	25.629	1.00	76.32	6
	ATOM	181	CB	GLN	A	235	20.328	25.239	24.391	1.00	76.98	6
	ATOM	182	CG	GLN	A	235	18.887	25.292	23.908	1.00	77.07	6
45	ATOM	183	CD	GLN	A	235	17.896	25.420	25.019	1.00	80.85	6
	ATOM	184	OE1	GLN	A	235	17.668	24.448	25.768	1.00	82.01	8
	ATOM	185	NE2	GLN	A	235	17.313	26.596	25.149	1.00	78.80	7
	ATOM	186	C	GLN	A	235	21.960	23.840	25.573	1.00	77.15	6
	ATOM	187	O	GLN	A	235	22.386	23.458	24.508	1.00	76.06	8
50	ATOM	188	N	GLY	A	236	22.676	23.766	26.687	1.00	77.46	7
	ATOM	189	CA	GLY	A	236	24.053	23.245	26.627	1.00	78.37	6
	ATOM	190	C	GLY	A	236	24.923	23.491	25.390	1.00	79.43	6
	ATOM	191	O	GLY	A	236	24.917	24.565	24.844	1.00	79.47	8
	ATOM	192	N	SER	A	237	25.739	22.526	24.991	1.00	77.98	7
55	ATOM	193	CA	SER	A	237	26.566	22.760	23.801	1.00	76.49	6
	ATOM	194	CB	SER	A	237	27.981	22.206	24.015	1.00	76.46	6
	ATOM	195	OG	SER	A	237	28.821	23.145	24.689	1.00	40.00	8
	ATOM	196	C	SER	A	237	25.938	22.127	22.542	1.00	75.35	6

5	ATOM	197	O	SER A 237	26.605	21.418	21.797	1.00	75.47	8
	ATOM	198	N	HIS A 238	24.648	22.410	22.353	1.00	75.56	7
	ATOM	199	CA	HIS A 238	23.842	21.981	21.236	1.00	75.46	6
	ATOM	200	CB	HIS A 238	22.990	20.732	21.661	1.00	75.85	6
	ATOM	201	CG	HIS A 238	22.408	19.933	20.542	1.00	40.00	6
10	ATOM	202	CD2	HIS A 238	22.790	18.757	19.957	1.00	40.00	6
	ATOM	203	ND1	HIS A 238	21.223	20.303	19.875	1.00	40.00	7
	ATOM	204	CE1	HIS A 238	20.951	19.365	18.953	1.00	40.00	6
	ATOM	205	NE2	HIS A 238	21.874	18.444	18.994	1.00	40.00	7
	ATOM	206	C	HIS A 238	22.971	23.284	20.964	1.00	74.10	6
15	ATOM	207	O	HIS A 238	21.863	23.137	20.441	1.00	75.34	8
	ATOM	208	N	TRP A 239	23.487	24.510	21.368	1.00	73.39	7
	ATOM	209	CA	TRP A 239	22.872	25.894	21.195	1.00	74.02	6
	ATOM	210	CB	TRP A 239	23.563	27.026	22.005	1.00	81.77	6
	ATOM	211	CG	TRP A 239	25.022	27.366	21.688	1.00	89.67	6
20	ATOM	212	CD2	TRP A 239	25.532	28.662	21.240	1.00	93.19	6
	ATOM	213	CE2	TRP A 239	26.961	28.522	21.136	1.00	95.46	6
	ATOM	214	CE3	TRP A 239	24.936	29.911	20.969	1.00	95.35	6
	ATOM	215	CD1	TRP A 239	26.102	26.548	21.781	1.00	94.16	6
	ATOM	216	NE1	TRP A 239	27.268	27.241	21.475	1.00	97.48	7
25	ATOM	217	CZ2	TRP A 239	27.798	29.598	20.764	1.00	96.23	6
	ATOM	218	CZ3	TRP A 239	25.763	30.967	20.569	1.00	96.75	6
	ATOM	219	CH2	TRP A 239	27.171	30.825	20.482	1.00	97.32	6
	ATOM	220	C	TRP A 239	22.799	26.407	19.774	1.00	70.77	6
	ATOM	221	O	TRP A 239	21.706	26.562	19.263	1.00	71.70	8
30	ATOM	222	N	LYS A 240	23.946	26.701	19.157	1.00	67.10	7
	ATOM	223	CA	LYS A 240	23.978	27.180	17.783	1.00	65.63	6
	ATOM	224	CB	LYS A 240	25.314	26.780	17.153	1.00	66.65	6
	ATOM	225	CG	LYS A 240	26.529	27.342	17.872	1.00	69.83	6
	ATOM	226	CD	LYS A 240	27.805	27.037	17.108	1.00	71.49	6
35	ATOM	227	CE	LYS A 240	28.980	27.720	17.776	1.00	71.31	6
	ATOM	228	NZ	LYS A 240	30.238	27.438	17.034	1.00	72.23	7
	ATOM	229	C	LYS A 240	22.808	26.699	16.895	1.00	66.19	6
	ATOM	230	O	LYS A 240	22.550	27.298	15.851	1.00	65.20	8
	ATOM	231	N	ASN A 241	22.113	25.640	17.325	1.00	66.69	7
40	ATOM	232	CA	ASN A 241	20.976	25.078	16.599	1.00	67.53	6
	ATOM	233	CB	ASN A 241	21.122	23.562	16.550	1.00	67.98	6
	ATOM	234	CG	ASN A 241	22.304	23.121	15.693	1.00	70.19	6
	ATOM	235	OD1	ASN A 241	22.404	23.506	14.503	1.00	71.37	8
	ATOM	236	ND2	ASN A 241	23.176	22.310	16.271	1.00	71.48	7
45	ATOM	237	C	ASN A 241	19.570	25.421	17.152	1.00	66.62	6
	ATOM	238	O	ASN A 241	18.581	24.822	16.731	1.00	64.76	8
	ATOM	239	N	LYS A 242	19.475	26.380	18.069	1.00	66.86	7
	ATOM	240	CA	LYS A 242	18.191	26.786	18.642	1.00	67.46	6
	ATOM	241	CB	LYS A 242	18.164	26.396	20.119	1.00	67.93	6
50	ATOM	242	CG	LYS A 242	18.250	24.896	20.337	1.00	71.52	6
	ATOM	243	CD	LYS A 242	17.004	24.149	19.821	1.00	74.32	6
	ATOM	244	CE	LYS A 242	15.755	24.491	20.643	1.00	74.41	6
	ATOM	245	NZ	LYS A 242	15.927	24.161	22.109	1.00	74.44	7
	ATOM	246	C	LYS A 242	18.143	28.291	18.483	1.00	66.28	6
55	ATOM	247	O	LYS A 242	17.102	28.923	18.592	1.00	67.61	8
	ATOM	248	N	ARG A 243	19.334	28.813	18.204	1.00	64.19	7
	ATOM	249	CA	ARG A 243	19.617	30.219	17.975	1.00	62.43	6
	ATOM	250	CB	ARG A 243	21.070	30.274	17.463	1.00	60.12	6

5	ATOM	251	CG	ARG	A	243	21.665	31.636	17.305	1.00	40.00	6
	ATOM	252	CD	ARG	A	243	23.213	31.599	17.267	1.00	40.00	6
	ATOM	253	NE	ARG	A	243	23.826	31.217	15.996	1.00	40.00	7
	ATOM	254	CZ	ARG	A	243	25.113	31.439	15.714	1.00	40.00	6
	ATOM	255	NH1	ARG	A	243	25.905	32.041	16.616	1.00	40.00	7
10	ATOM	256	NH2	ARG	A	243	25.592	31.097	14.520	1.00	40.00	7
	ATOM	257	C	ARG	A	243	18.639	30.789	16.950	1.00	62.97	6
	ATOM	258	O	ARG	A	243	18.662	30.390	15.784	1.00	63.96	8
	ATOM	259	N	LYS	A	244	17.771	31.692	17.393	1.00	62.41	7
	ATOM	260	CA	LYS	A	244	16.790	32.309	16.498	1.00	61.57	6
15	ATOM	261	CB	LYS	A	244	15.368	31.974	16.962	1.00	63.68	6
	ATOM	262	CG	LYS	A	244	15.102	30.471	17.104	1.00	71.29	6
	ATOM	263	CD	LYS	A	244	13.641	30.167	17.468	1.00	73.83	6
	ATOM	264	CE	LYS	A	244	13.182	30.908	18.737	1.00	74.71	6
	ATOM	265	NZ	LYS	A	244	13.951	30.536	19.970	1.00	73.32	7
20	ATOM	266	C	LYS	A	244	17.009	33.806	16.501	1.00	59.30	6
	ATOM	267	O	LYS	A	244	16.562	34.514	17.399	1.00	56.34	8
	ATOM	268	N	PHE	A	245	17.705	34.264	15.468	1.00	57.06	7
	ATOM	269	CA	PHE	A	245	18.045	35.692	15.333	1.00	59.01	6
	ATOM	270	CB	PHE	A	245	18.825	35.947	14.049	1.00	59.62	6
25	ATOM	271	CG	PHE	A	245	19.908	34.979	13.834	1.00	66.60	6
	ATOM	272	CD1	PHE	A	245	19.618	33.714	13.399	1.00	67.17	6
	ATOM	273	CD2	PHE	A	245	21.198	35.309	14.139	1.00	69.25	6
	ATOM	274	CE1	PHE	A	245	20.614	32.794	13.255	1.00	69.92	6
	ATOM	275	CE2	PHE	A	245	22.189	34.385	13.994	1.00	70.50	6
30	ATOM	276	CZ	PHE	A	245	21.897	33.126	13.552	1.00	70.89	6
	ATOM	277	C	PHE	A	245	16.856	36.620	15.340	1.00	60.68	6
	ATOM	278	O	PHE	A	245	15.946	36.516	14.528	1.00	62.37	8
	ATOM	279	N	LEU	A	246	16.919	37.558	16.272	1.00	60.10	7
	ATOM	280	CA	LEU	A	246	15.884	38.554	16.437	1.00	59.44	6
35	ATOM	281	CB	LEU	A	246	16.227	39.510	17.585	1.00	57.43	6
	ATOM	282	CG	LEU	A	246	15.100	40.384	18.086	1.00	54.41	6
	ATOM	283	CD1	LEU	A	246	14.010	39.474	18.640	1.00	52.43	6
	ATOM	284	CD2	LEU	A	246	15.575	41.325	19.151	1.00	51.69	6
	ATOM	285	C	LEU	A	246	15.717	39.330	15.135	1.00	62.05	6
40	ATOM	286	O	LEU	A	246	16.706	39.609	14.430	1.00	59.85	8
	ATOM	287	N	PRO	A	247	14.473	39.668	14.784	1.00	63.33	7
	ATOM	288	CD	PRO	A	247	13.263	39.314	15.534	1.00	64.44	6
	ATOM	289	CA	PRO	A	247	14.198	40.421	13.558	1.00	63.56	6
	ATOM	290	CB	PRO	A	247	12.687	40.671	13.600	1.00	64.42	6
45	ATOM	291	CG	PRO	A	247	12.161	39.922	14.729	1.00	64.90	6
	ATOM	292	C	PRO	A	247	14.996	41.733	13.496	1.00	61.94	6
	ATOM	293	O	PRO	A	247	15.159	42.455	14.486	1.00	61.60	8
	ATOM	294	N	GLU	A	248	15.506	42.006	12.299	1.00	61.33	7
	ATOM	295	CA	GLU	A	248	16.280	43.197	11.976	1.00	63.50	6
50	ATOM	296	CB	GLU	A	248	16.481	43.273	10.437	1.00	66.94	6
	ATOM	297	CG	GLU	A	248	17.012	44.671	9.966	1.00	68.70	6
	ATOM	298	CD	GLU	A	248	16.981	44.939	8.471	1.00	40.00	6
	ATOM	299	OE1	GLU	A	248	16.432	44.144	7.644	1.00	40.00	8
	ATOM	300	OE2	GLU	A	248	17.509	46.015	8.086	1.00	40.00	8
55	ATOM	301	C	GLU	A	248	15.624	44.489	12.458	1.00	64.19	6
	ATOM	302	O	GLU	A	248	16.298	45.395	12.918	1.00	65.56	8
	ATOM	303	N	ASP	A	249	14.300	44.545	12.323	1.00	64.36	7
	ATOM	304	CA	ASP	A	249	13.493	45.703	12.673	1.00	63.33	6

5	ATOM	305	CB	ASP	A	249	12.088	45.531	12.116	1.00	62.97	6
	ATOM	306	CG	ASP	A	249	11.277	44.527	12.870	1.00	64.63	6
	ATOM	307	OD1	ASP	A	249	11.687	43.352	12.963	1.00	64.84	8
	ATOM	308	OD2	ASP	A	249	10.183	44.880	13.395	1.00	66.52	8
	ATOM	309	C	ASP	A	249	13.371	46.062	14.130	1.00	64.31	6
10	ATOM	310	O	ASP	A	249	13.310	47.250	14.468	1.00	64.73	8
	ATOM	311	N	ILE	A	250	13.274	45.049	14.997	1.00	63.09	7
	ATOM	312	CA	ILE	A	250	13.133	45.318	16.418	1.00	64.39	6
	ATOM	313	CB	ILE	A	250	13.035	44.034	17.214	1.00	65.79	6
	ATOM	314	CG2	ILE	A	250	12.001	44.104	18.336	1.00	64.78	6
15	ATOM	315	CG1	ILE	A	250	12.611	42.860	16.341	1.00	65.28	6
	ATOM	316	CD1	ILE	A	250	11.753	41.852	17.088	1.00	65.08	6
	ATOM	317	C	ILE	A	250	14.404	46.104	17.276	1.00	65.21	6
	ATOM	318	O	ILE	A	250	15.155	45.506	18.047	1.00	64.05	8
	ATOM	319	N	GLY	A	251	14.670	47.529	17.299	1.00	65.48	7
20	ATOM	320	CA	GLY	A	251	15.871	48.326	18.042	1.00	67.32	6
	ATOM	321	C	GLY	A	251	16.595	49.110	16.895	1.00	68.52	6
	ATOM	322	O	GLY	A	251	17.528	48.616	16.266	1.00	65.49	8
	ATOM	323	N	GLN	A	252	16.162	50.356	16.557	1.00	72.26	7
	ATOM	324	CA	GLN	A	252	16.541	50.930	15.207	1.00	74.10	6
25	ATOM	325	CB	GLN	A	252	15.316	50.844	14.295	1.00	75.82	6
	ATOM	326	C	GLN	A	252	16.995	52.403	15.084	1.00	77.17	6
	ATOM	327	O	GLN	A	252	17.572	52.955	15.986	1.00	76.50	8
	ATOM	328	N	ALA	A	253	16.374	53.372	13.908	1.00	80.78	7
	ATOM	329	CA	ALA	A	253	16.687	54.725	13.567	1.00	83.70	6
30	ATOM	330	CE	ALA	A	253	16.381	54.956	12.093	1.00	83.23	6
	ATOM	331	C	ALA	A	253	16.159	55.960	14.345	1.00	85.59	6
	ATOM	332	O	ALA	A	253	15.317	56.721	13.798	1.00	85.69	8
	ATOM	333	N	PRO	A	254	16.384	56.155	16.264	1.00	35.05	7
	ATOM	334	CD	PRO	A	254	17.102	55.053	16.908	1.00	33.97	6
35	ATOM	335	CA	PRO	A	254	16.002	57.231	17.219	1.00	35.89	6
	ATOM	336	CB	PRO	A	254	16.534	56.756	18.563	1.00	33.94	6
	ATOM	337	CG	PRO	A	254	17.146	55.441	18.349	1.00	33.31	6
	ATOM	338	C	PRO	A	254	16.717	58.498	16.731	1.00	37.75	6
	ATOM	339	O	PRO	A	254	17.838	58.804	17.100	1.00	38.78	8
40	TER											
	ATOM	1	N	LYS	A	263	18.045	57.462	23.875	1.00	61.71	7
	ATOM	2	CA	LYS	A	263	16.824	56.712	24.215	1.00	64.36	6
	ATOM	3	CB	LYS	A	263	15.758	57.004	23.141	1.00	63.50	6
	ATOM	4	C	LYS	A	263	16.841	55.180	24.429	1.00	63.41	6
45	ATOM	5	O	LYS	A	263	17.877	54.542	24.409	1.00	61.93	8
	ATOM	6	N	VAL	A	264	15.615	54.664	24.654	1.00	61.15	7
	ATOM	7	CA	VAL	A	264	15.292	53.229	24.856	1.00	59.46	6
	ATOM	8	CB	VAL	A	264	14.251	52.974	25.978	1.00	59.03	6
	ATOM	9	CG1	VAL	A	264	14.229	51.494	26.368	1.00	53.79	6
50	ATOM	10	CG2	VAL	A	264	14.449	53.818	27.142	1.00	55.32	6
	ATOM	11	C	VAL	A	264	14.590	52.820	23.554	1.00	60.96	6
	ATOM	12	O	VAL	A	264	14.734	53.468	22.508	1.00	62.13	8
	ATOM	13	N	ASP	A	265	13.802	51.755	23.634	1.00	62.59	7
	ATOM	14	CA	ASP	A	265	12.995	51.263	22.526	1.00	64.95	6
55	ATOM	15	CB	ASP	A	265	13.825	51.077	21.271	1.00	64.32	6
	ATOM	16	CG	ASP	A	265	13.282	50.048	20.485	1.00	67.70	6
	ATOM	17	OD1	ASP	A	265	12.795	50.011	19.446	1.00	72.59	8
	ATOM	18	OD2	ASP	A	265	13.354	48.867	20.294	1.00	68.84	8

5	ATOM	19	C	ASP	A	265	12.326	49.943	22.952	1.00	65.64	6
	ATOM	20	O	ASP	A	265	12.771	48.850	22.655	1.00	68.81	8
	ATOM	21	N	LEU	A	266	11.256	50.152	23.702	1.00	65.12	7
	ATOM	22	CA	LEU	A	266	10.368	49.169	24.288	1.00	63.40	6
	ATOM	23	CB	LEU	A	266	9.115	49.938	24.708	1.00	67.34	6
10	ATOM	24	CG	LEU	A	266	9.399	51.124	25.618	1.00	69.35	6
	ATOM	25	CD1	LEU	A	266	8.304	52.148	25.533	1.00	68.24	6
	ATOM	26	CD2	LEU	A	266	9.581	50.631	27.021	1.00	70.47	6
	ATOM	27	C	LEU	A	266	9.940	47.888	23.559	1.00	59.67	6
	ATOM	28	O	LEU	A	266	9.694	46.879	24.220	1.00	53.35	8
15	ATOM	29	N	GLU	A	267	9.815	47.904	22.235	1.00	58.01	7
	ATOM	30	CA	GLU	A	267	9.417	46.682	21.572	1.00	58.34	6
	ATOM	31	CB	GLU	A	267	9.311	46.855	20.048	1.00	59.21	6
	ATOM	32	CG	GLU	A	267	9.129	45.494	19.322	1.00	62.89	6
	ATOM	33	CD	GLU	A	267	8.736	45.592	17.883	1.00	67.66	6
20	ATOM	34	OE1	GLU	A	267	9.433	46.263	17.080	1.00	69.95	8
	ATOM	35	OE2	GLU	A	267	7.710	44.974	17.503	1.00	69.40	8
	ATOM	36	C	GLU	A	267	10.504	45.683	21.895	1.00	57.67	6
	ATOM	37	O	GLU	A	267	10.255	44.485	21.988	1.00	58.34	8
	ATOM	38	N	ALA	A	268	11.712	46.222	22.054	1.00	53.43	7
25	ATOM	39	CA	ALA	A	268	12.903	45.454	22.374	1.00	49.00	6
	ATOM	40	CB	ALA	A	268	14.137	46.241	21.983	1.00	45.72	6
	ATOM	41	C	ALA	A	268	12.908	45.196	23.873	1.00	45.76	6
	ATOM	42	O	ALA	A	268	12.887	44.042	24.307	1.00	41.50	8
	ATOM	43	N	PHE	A	269	12.918	46.277	24.663	1.00	41.43	7
30	ATOM	44	CA	PHE	A	269	12.920	46.158	26.118	1.00	43.96	6
	ATOM	45	CB	PHE	A	269	12.395	47.426	26.777	1.00	40.10	6
	ATOM	46	CG	PHE	A	269	12.332	47.345	28.271	1.00	40.44	6
	ATOM	47	CD1	PHE	A	269	13.457	47.595	29.034	1.00	38.98	6
	ATOM	48	CD2	PHE	A	269	11.165	46.946	28.903	1.00	37.15	6
35	ATOM	49	CE1	PHE	A	269	13.409	47.469	30.436	1.00	32.12	6
	ATOM	50	CE2	PHE	A	269	11.105	46.815	30.303	1.00	38.41	6
	ATOM	51	CZ	PHE	A	269	12.228	47.070	31.071	1.00	40.55	6
	ATOM	52	C	PHE	A	269	12.017	45.012	26.520	1.00	49.76	6
	ATOM	53	O	PHE	A	269	12.277	44.324	27.484	1.00	52.15	8
40	ATOM	54	N	SER	A	270	10.934	44.835	25.768	1.00	53.15	7
	ATOM	55	CA	SER	A	270	9.988	43.768	26.043	1.00	52.29	6
	ATOM	56	CB	SER	A	270	8.727	43.943	25.215	1.00	51.85	6
	ATOM	57	OG	SER	A	270	7.785	42.918	25.497	1.00	53.42	8
	ATOM	58	C	SER	A	270	10.637	42.464	25.685	1.00	49.38	6
45	ATOM	59	O	SER	A	270	11.068	41.741	26.562	1.00	48.74	8
	ATOM	60	N	HIS	A	271	10.683	42.173	24.383	1.00	50.15	7
	ATOM	61	CA	HIS	A	271	11.276	40.932	23.877	1.00	51.67	6
	ATOM	62	CB	HIS	A	271	11.797	41.118	22.455	1.00	58.52	6
	ATOM	63	CG	HIS	A	271	10.775	40.885	21.399	1.00	68.97	6
50	ATOM	64	CD2	HIS	A	271	10.633	39.891	20.485	1.00	70.88	6
	ATOM	65	ND1	HIS	A	271	9.673	41.732	21.199	1.00	71.98	7
	ATOM	66	CE1	HIS	A	271	8.936	41.242	20.209	1.00	73.91	6
	ATOM	67	NE2	HIS	A	271	9.495	40.132	19.764	1.00	73.59	7
	ATOM	68	C	HIS	A	271	12.402	40.416	24.745	1.00	48.33	6
55	ATOM	69	O	HIS	A	271	12.707	39.225	24.728	1.00	48.39	8
	ATOM	70	N	PHE	A	272	13.029	41.334	25.487	1.00	41.34	7
	ATOM	71	CA	PHE	A	272	14.130	41.001	26.384	1.00	39.44	6
	ATOM	72	CB	PHE	A	272	15.077	42.194	26.512	1.00	36.67	6

5	ATOM	73	CG	PHE	A	272	15.953	42.413	25.282	1.00	33.39	6
	ATOM	74	CD1	PHE	A	272	16.619	43.615	25.093	1.00	33.14	6
	ATOM	75	CD2	PHE	A	272	16.138	41.394	24.346	1.00	38.28	6
	ATOM	76	CE1	PHE	A	272	17.454	43.807	23.988	1.00	38.26	6
	ATOM	77	CE2	PHE	A	272	16.973	41.585	23.244	1.00	43.28	6
10	ATOM	78	CZ	PHE	A	272	17.634	42.786	23.068	1.00	39.74	6
	ATOM	79	C	PHE	A	272	13.650	40.528	27.764	1.00	40.75	6
	ATOM	80	O	PHE	A	272	14.081	39.476	28.227	1.00	35.51	8
	ATOM	81	N	THR	A	273	12.756	41.266	28.428	1.00	41.64	7
	ATOM	82	CA	THR	A	273	12.290	40.854	29.757	1.00	45.97	6
15	ATOM	83	CB	THR	A	273	11.651	42.025	30.506	1.00	51.52	6
	ATOM	84	OG1	THR	A	273	10.442	42.422	29.859	1.00	45.74	8
	ATOM	85	CG2	THR	A	273	12.601	43.211	30.565	1.00	49.73	6
	ATOM	86	C	THR	A	273	11.267	39.731	29.664	1.00	46.23	6
	ATOM	87	O	THR	A	273	10.854	39.183	30.680	1.00	41.21	8
20	ATOM	88	N	LYS	A	274	10.849	39.412	28.440	1.00	46.21	7
	ATOM	89	CA	LYS	A	274	9.871	38.362	28.211	1.00	54.53	6
	ATOM	90	CB	LYS	A	274	9.414	38.405	26.773	1.00	54.36	6
	ATOM	91	C	LYS	A	274	10.498	37.015	28.515	1.00	56.88	6
	ATOM	92	O	LYS	A	274	9.789	36.044	28.759	1.00	57.98	8
25	ATOM	93	N	ILE	A	275	11.836	36.973	28.491	1.00	56.48	7
	ATOM	94	CA	ILE	A	275	12.609	35.746	28.767	1.00	52.64	6
	ATOM	95	CB	ILE	A	275	13.444	35.346	27.543	1.00	49.15	6
	ATOM	96	CG2	ILE	A	275	12.568	34.829	26.429	1.00	47.42	6
	ATOM	97	CG1	ILE	A	275	14.238	36.532	27.026	1.00	45.31	6
30	ATOM	98	CD1	ILE	A	275	15.001	36.242	25.771	1.00	37.22	6
	ATOM	99	C	ILE	A	275	13.541	35.870	29.982	1.00	51.78	6
	ATOM	100	O	ILE	A	275	14.014	34.873	30.503	1.00	49.80	8
	ATOM	101	N	ILE	A	276	13.790	37.107	30.415	1.00	51.76	7
	ATOM	102	CA	ILE	A	276	14.681	37.389	31.537	1.00	52.58	6
35	ATOM	103	CB	ILE	A	276	14.691	38.877	31.844	1.00	55.04	6
	ATOM	104	CG2	ILE	A	276	13.311	39.340	32.261	1.00	53.28	6
	ATOM	105	CG1	ILE	A	276	15.675	39.206	32.976	1.00	57.31	6
	ATOM	106	CD1	ILE	A	276	17.096	38.942	32.655	1.00	60.32	6
	ATOM	107	C	ILE	A	276	14.323	36.644	32.828	1.00	50.70	6
40	ATOM	108	O	ILE	A	276	15.177	36.458	33.691	1.00	55.55	8
	ATOM	109	N	THR	A	277	13.072	36.209	32.963	1.00	47.33	7
	ATOM	110	CA	THR	A	277	12.631	35.523	34.158	1.00	42.59	6
	ATOM	111	CB	THR	A	277	11.098	35.456	34.217	1.00	44.97	6
	ATOM	112	OG1	THR	A	277	10.545	36.777	34.102	1.00	46.38	8
45	ATOM	113	CG2	THR	A	277	10.657	34.838	35.539	1.00	37.17	6
	ATOM	114	C	THR	A	277	13.211	34.118	34.304	1.00	39.84	6
	ATOM	115	O	THR	A	277	13.796	33.796	35.365	1.00	40.55	8
	ATOM	116	N	PRO	A	278	13.055	33.261	33.288	1.00	38.20	7
	ATOM	117	CD	PRO	A	278	12.370	33.534	32.023	1.00	36.34	6
50	ATOM	118	CA	PRO	A	278	13.595	31.894	33.363	1.00	36.63	6
	ATOM	119	CB	PRO	A	278	13.153	31.244	32.064	1.00	32.95	6
	ATOM	120	CG	PRO	A	278	12.573	32.291	31.239	1.00	35.75	6
	ATOM	121	C	PRO	A	278	15.101	31.932	33.476	1.00	38.60	6
	ATOM	122	O	PRO	A	278	15.746	30.981	33.898	1.00	37.67	8
55	ATOM	123	N	ALA	A	279	15.656	33.051	33.035	1.00	37.05	7
	ATOM	124	CA	ALA	A	279	17.087	33.277	33.041	1.00	33.18	6
	ATOM	125	CB	ALA	A	279	17.376	34.599	32.348	1.00	30.56	6
	ATOM	126	C	ALA	A	279	17.624	33.312	34.452	1.00	33.47	6

5	ATOM	127	O	ALA	A	279	18.523	32.555	34.789	1.00	33.74	8
	ATOM	128	N	ILE	A	280	17.060	34.215	35.260	1.00	29.96	7
	ATOM	129	CA	ILE	A	280	17.459	34.362	36.646	1.00	25.94	6
	ATOM	130	CB	ILE	A	280	16.686	35.484	37.315	1.00	26.95	6
	ATOM	131	CG2	ILE	A	280	17.109	35.632	38.733	1.00	15.40	6
10	ATOM	132	CG1	ILE	A	280	16.931	36.808	36.595	1.00	26.73	6
	ATOM	133	CD1	ILE	A	280	16.292	38.002	37.272	1.00	34.31	6
	ATOM	134	C	ILE	A	280	17.263	33.066	37.412	1.00	31.39	6
	ATOM	135	O	ILE	A	280	18.116	32.679	38.207	1.00	35.69	8
	ATOM	136	N	THR	A	281	16.145	32.386	37.165	1.00	30.90	7
15	ATOM	137	CA	THR	A	281	15.854	31.118	37.851	1.00	33.49	6
	ATOM	138	CB	THR	A	281	14.598	30.413	37.277	1.00	37.18	6
	ATOM	139	OG1	THR	A	281	14.795	30.099	35.898	1.00	46.48	8
	ATOM	140	CG2	THR	A	281	13.352	31.281	37.444	1.00	32.85	6
	ATOM	141	C	THR	A	281	17.045	30.176	37.713	1.00	29.94	6
20	ATOM	142	O	THR	A	281	17.478	29.546	38.684	1.00	25.55	8
	ATOM	143	N	ARG	A	282	17.561	30.076	36.489	1.00	32.70	7
	ATOM	144	CA	ARG	A	282	18.692	29.198	36.218	1.00	34.27	6
	ATOM	145	CB	ARG	A	282	19.136	29.374	34.780	1.00	33.78	6
	ATOM	146	CG	ARG	A	282	19.272	28.086	34.013	1.00	45.15	6
25	ATOM	147	CD	ARG	A	282	18.179	27.921	32.977	1.00	58.24	6
	ATOM	148	NE	ARG	A	282	18.041	29.077	32.117	1.00	68.41	7
	ATOM	149	CZ	ARG	A	282	19.018	29.529	31.352	1.00	72.31	6
	ATOM	150	NH1	ARG	A	282	20.190	28.886	31.327	1.00	77.89	7
	ATOM	151	NH2	ARG	A	282	18.802	30.593	30.595	1.00	69.25	7
30	ATOM	152	C	ARG	A	282	19.823	29.582	37.170	1.00	34.81	6
	ATOM	153	O	ARG	A	282	20.380	28.735	37.855	1.00	36.03	8
	ATOM	154	N	VAL	A	283	20.135	30.882	37.190	1.00	31.71	7
	ATOM	155	CA	VAL	A	283	21.171	31.434	38.057	1.00	30.16	6
	ATOM	156	CB	VAL	A	283	21.198	32.965	37.981	1.00	29.00	6
35	ATOM	157	CG1	VAL	A	283	22.208	33.533	38.952	1.00	28.64	6
	ATOM	158	CG2	VAL	A	283	21.525	33.415	36.578	1.00	28.28	6
	ATOM	159	C	VAL	A	283	20.942	30.992	39.498	1.00	32.50	6
	ATOM	160	O	VAL	A	283	21.879	30.717	40.229	1.00	33.48	8
	ATOM	161	N	VAL	A	284	19.671	30.941	39.892	1.00	30.96	7
40	ATOM	162	CA	VAL	A	284	19.289	30.527	41.239	1.00	29.14	6
	ATOM	163	CB	VAL	A	284	17.822	30.865	41.548	1.00	31.27	6
	ATOM	164	CG1	VAL	A	284	17.472	30.461	42.945	1.00	24.21	6
	ATOM	165	CG2	VAL	A	284	17.555	32.334	41.360	1.00	30.51	6
	ATOM	166	C	VAL	A	284	19.529	29.037	41.353	1.00	28.89	6
45	ATOM	167	O	VAL	A	284	20.073	28.568	42.345	1.00	27.29	8
	ATOM	168	N	ASP	A	285	19.121	28.296	40.327	1.00	28.76	7
	ATOM	169	CA	ASP	A	285	19.277	26.842	40.306	1.00	35.32	6
	ATOM	170	CB	ASP	A	285	18.586	26.234	39.072	1.00	33.29	6
	ATOM	171	CG	ASP	A	285	17.083	26.277	39.149	1.00	38.15	6
50	ATOM	172	OD1	ASP	A	285	16.484	25.743	40.110	1.00	34.70	8
	ATOM	173	OD2	ASP	A	285	16.431	26.828	38.231	1.00	34.43	8
	ATOM	174	C	ASP	A	285	20.751	26.449	40.305	1.00	36.70	6
	ATOM	175	O	ASP	A	285	21.106	25.389	40.808	1.00	37.96	8
	ATOM	176	N	PHE	A	286	21.604	27.300	39.737	1.00	35.96	7
55	ATOM	177	CA	PHE	A	286	23.029	27.022	39.704	1.00	37.10	6
	ATOM	178	CB	PHE	A	286	23.754	28.009	38.793	1.00	37.97	6
	ATOM	179	CG	PHE	A	286	25.252	28.027	38.987	1.00	36.50	6
	ATOM	180	CD1	PHE	A	286	25.963	26.849	38.974	1.00	36.75	6



5	ATOM	181	CD2	PHE	A	286	25.931	29.218	39.199	1.00	33.83	6
	ATOM	182	CE1	PHE	A	286	27.331	26.860	39.161	1.00	39.55	6
	ATOM	183	CE2	PHE	A	286	27.307	29.233	39.387	1.00	38.08	6
	ATOM	184	CZ	PHE	A	286	28.008	28.052	39.371	1.00	34.44	6
	ATOM	185	C	PHE	A	286	23.631	27.105	41.083	1.00	36.83	6
10	ATOM	186	O	PHE	A	286	24.317	26.192	41.504	1.00	35.61	8
	ATOM	187	N	ALA	A	287	23.393	28.228	41.752	1.00	37.33	7
	ATOM	188	CA	ALA	A	287	23.917	28.448	43.087	1.00	36.34	6
	ATOM	189	CB	ALA	A	287	23.523	29.828	43.555	1.00	36.40	6
	ATOM	190	C	ALA	A	287	23.346	27.393	44.027	1.00	38.76	6
15	ATOM	191	O	ALA	A	287	23.994	26.973	44.981	1.00	41.98	8
	ATOM	192	N	LYS	A	288	22.114	26.979	43.735	1.00	38.28	7
	ATOM	193	CA	LYS	A	288	21.429	25.971	44.538	1.00	45.26	6
	ATOM	194	CB	LYS	A	288	19.994	25.746	44.054	1.00	48.35	6
	ATOM	195	CG	LYS	A	288	19.025	26.819	44.464	1.00	51.43	6
20	ATOM	196	CD	LYS	A	288	17.628	26.246	44.682	1.00	60.23	6
	ATOM	197	CE	LYS	A	288	17.135	25.478	43.485	1.00	62.81	6
	ATOM	198	NZ	LYS	A	288	17.196	26.327	42.268	1.00	64.69	7
	ATOM	199	C	LYS	A	288	22.120	24.632	44.536	1.00	43.31	6
	ATOM	200	O	LYS	A	288	21.967	23.857	45.462	1.00	45.66	8
25	ATOM	201	N	LYS	A	289	22.865	24.366	43.467	1.00	41.70	7
	ATOM	202	CA	LYS	A	289	23.571	23.120	43.351	1.00	40.67	6
	ATOM	203	CB	LYS	A	289	23.655	22.708	41.877	1.00	42.25	6
	ATOM	204	CG	LYS	A	289	22.271	22.492	41.247	1.00	39.53	6
	ATOM	205	CD	LYS	A	289	22.331	21.606	40.012	1.00	43.19	6
30	ATOM	206	CE	LYS	A	289	20.941	21.362	39.447	1.00	45.74	6
	ATOM	207	NZ	LYS	A	289	20.273	20.165	40.006	1.00	52.49	7
	ATOM	208	C	LYS	A	289	24.948	23.185	44.003	1.00	41.50	6
	ATOM	209	O	LYS	A	289	25.642	22.184	44.080	1.00	39.77	8
	ATOM	210	N	LEU	A	290	25.312	24.370	44.490	1.00	40.68	7
35	ATOM	211	CA	LEU	A	290	26.594	24.583	45.149	1.00	39.33	6
	ATOM	212	CB	LEU	A	290	27.153	25.972	44.829	1.00	36.14	6
	ATOM	213	CG	LEU	A	290	27.358	26.290	43.365	1.00	34.81	6
	ATOM	214	CD1	LEU	A	290	27.945	27.675	43.208	1.00	29.07	6
	ATOM	215	CD2	LEU	A	290	28.267	25.242	42.757	1.00	33.45	6
40	ATOM	216	C	LEU	A	290	26.434	24.405	46.652	1.00	40.08	6
	ATOM	217	O	LEU	A	290	25.803	25.235	47.333	1.00	42.00	8
	ATOM	218	N	PRO	A	291	27.028	23.333	47.210	1.00	40.27	7
	ATOM	219	CD	PRO	A	291	27.851	22.330	46.519	1.00	39.65	6
	ATOM	220	CA	PRO	A	291	26.905	23.096	48.659	1.00	38.28	6
45	ATOM	221	CB	PRO	A	291	27.755	21.860	48.911	1.00	35.88	6
	ATOM	222	CG	PRO	A	291	28.202	21.355	47.585	1.00	34.19	6
	ATOM	223	C	PRO	A	291	27.327	24.298	49.522	1.00	40.05	6
	ATOM	224	O	PRO	A	291	26.571	24.739	50.391	1.00	41.33	8
	ATOM	225	N	MET	A	292	28.522	24.843	49.299	1.00	40.59	7
50	ATOM	226	CA	MET	A	292	29.021	25.957	50.097	1.00	42.86	6
	ATOM	227	CB	MET	A	292	30.313	26.475	49.477	1.00	43.28	6
	ATOM	228	CG	MET	A	292	31.269	25.378	49.050	1.00	50.35	6
	ATOM	229	SD	MET	A	292	32.895	26.096	48.757	1.00	51.17	16
	ATOM	230	CE	MET	A	292	33.812	24.647	48.074	1.00	54.63	6
55	ATOM	231	C	MET	A	292	27.984	27.066	50.149	1.00	41.05	6
	ATOM	232	O	MET	A	292	27.986	27.886	51.057	1.00	39.66	8
	ATOM	233	N	PHE	A	293	27.080	27.078	49.172	1.00	39.30	7
	ATOM	234	CA	PHE	A	293	26.030	28.091	49.114	1.00	40.92	6

5	ATOM	235	CB	PHE A 293	25.398	28.107	47.715	1.00	40.98	6
	ATOM	236	CG	PHE A 293	24.348	29.168	47.524	1.00	42.78	6
	ATOM	237	CD1	PHE A 293	24.654	30.493	47.747	1.00	44.40	6
	ATOM	238	CD2	PHE A 293	23.071	28.833	47.116	1.00	43.66	6
	ATOM	239	CE1	PHE A 293	23.701	31.478	47.564	1.00	39.83	6
10	ATOM	240	CE2	PHE A 293	22.112	29.819	46.930	1.00	46.21	6
	ATOM	241	CZ	PHE A 293	22.430	31.146	47.155	1.00	45.18	6
	ATOM	242	C	PHE A 293	24.979	27.772	50.164	1.00	45.54	6
	ATOM	243	O	PHE A 293	24.686	28.576	51.034	1.00	42.01	8
	ATOM	244	N	CYS A 294	24.426	26.572	50.062	1.00	47.05	7
15	ATOM	245	CA	CYS A 294	23.386	26.125	50.962	1.00	50.15	6
	ATOM	246	CB	CYS A 294	22.944	24.733	50.524	1.00	45.90	6
	ATOM	247	SG	CYS A 294	22.303	24.663	48.829	1.00	51.50	16
	ATOM	248	C	CYS A 294	23.825	26.125	52.423	1.00	51.38	6
	ATOM	249	O	CYS A 294	23.008	25.954	53.322	1.00	53.83	8
20	ATOM	250	N	GLU A 295	25.119	26.327	52.645	1.00	49.72	7
	ATOM	251	CA	GLU A 295	25.666	26.384	53.996	1.00	52.53	6
	ATOM	252	CB	GLU A 295	27.103	25.830	54.015	1.00	57.40	6
	ATOM	253	CG	GLU A 295	27.182	24.309	54.061	1.00	69.63	6
	ATOM	254	CD	GLU A 295	26.660	23.747	55.342	1.00	78.49	6
25	ATOM	255	OE1	GLU A 295	27.291	23.946	56.412	1.00	82.82	8
	ATOM	256	OE2	GLU A 295	25.590	23.086	55.335	1.00	85.30	8
	ATOM	257	C	GLU A 295	25.653	27.831	54.488	1.00	48.54	6
	ATOM	258	O	GLU A 295	26.365	28.184	55.426	1.00	49.82	8
	ATOM	259	N	LEU A 296	24.804	28.631	53.846	1.00	43.79	7
30	ATOM	260	CA	LEU A 296	24.670	30.034	54.159	1.00	45.42	6
	ATOM	261	CB	LEU A 296	25.062	30.864	52.923	1.00	41.04	6
	ATOM	262	CG	LEU A 296	26.438	30.658	52.315	1.00	42.74	6
	ATOM	263	CD1	LEU A 296	26.447	31.030	50.861	1.00	40.99	6
	ATOM	264	CD2	LEU A 296	27.437	31.454	53.086	1.00	39.44	6
35	ATOM	265	C	LEU A 296	23.239	30.366	54.548	1.00	45.56	6
	ATOM	266	O	LEU A 296	22.301	29.660	54.148	1.00	43.07	8
	ATOM	267	N	PRO A 297	23.050	31.405	55.365	1.00	46.99	7
	ATOM	268	CD	PRO A 297	24.121	32.241	55.930	1.00	47.12	6
	ATOM	269	CA	PRO A 297	21.700	31.811	55.787	1.00	49.61	6
40	ATOM	270	CB	PRO A 297	21.937	32.990	56.738	1.00	49.91	6
	ATOM	271	CG	PRO A 297	23.401	33.155	56.872	1.00	51.28	6
	ATOM	272	C	PRO A 297	20.864	32.212	54.558	1.00	49.59	6
	ATOM	273	O	PRO A 297	21.402	32.684	53.556	1.00	51.66	8
	ATOM	274	N	CYS A 298	19.545	32.035	54.655	1.00	51.02	7
45	ATOM	275	CA	CYS A 298	18.618	32.369	53.567	1.00	52.86	6
	ATOM	276	CB	CYS A 298	17.201	31.877	53.915	1.00	54.57	6
	ATOM	277	SG	CYS A 298	16.040	33.162	54.440	1.00	67.87	16
	ATOM	278	C	CYS A 298	18.583	33.863	53.291	1.00	48.51	6
	ATOM	279	O	CYS A 298	18.039	34.288	52.282	1.00	49.58	8
50	ATOM	280	N	GLU A 299	19.144	34.654	54.202	1.00	44.17	7
	ATOM	281	CA	GLU A 299	19.179	36.096	54.016	1.00	47.57	6
	ATOM	282	CB	GLU A 299	19.265	36.833	55.360	1.00	49.92	6
	ATOM	283	CG	GLU A 299	17.931	36.996	56.125	1.00	59.30	6
	ATOM	284	CD	GLU A 299	17.613	35.904	57.095	1.00	63.80	6
55	ATOM	285	OE1	GLU A 299	16.512	35.952	57.706	1.00	69.03	8
	ATOM	286	OE2	GLU A 299	18.436	34.976	57.292	1.00	67.10	8
	ATOM	287	C	GLU A 299	20.359	36.492	53.152	1.00	46.57	6
	ATOM	288	O	GLU A 299	20.265	37.441	52.379	1.00	44.65	8

5	ATOM	289	N	ASP	A	300	21.467	35.765	53.294	1.00	45.17	7
	ATOM	290	CA	ASP	A	300	22.661	36.042	52.509	1.00	43.32	6
	ATOM	291	CB	ASP	A	300	23.919	35.513	53.213	1.00	37.38	6
	ATOM	292	CG	ASP	A	300	24.223	36.239	54.473	1.00	36.23	6
	ATOM	293	OD1	ASP	A	300	24.153	37.488	54.493	1.00	35.87	8
10	ATOM	294	OD2	ASP	A	300	24.572	35.575	55.483	1.00	40.14	8
	ATOM	295	C	ASP	A	300	22.514	35.390	51.138	1.00	42.81	6
	ATOM	296	O	ASP	A	300	22.775	36.021	50.113	1.00	46.02	8
	ATOM	297	N	GLN	A	301	22.095	34.124	51.137	1.00	38.60	7
	ATOM	298	CA	GLN	A	301	21.896	33.390	49.902	1.00	40.00	6
15	ATOM	299	CB	GLN	A	301	20.991	32.179	50.137	1.00	38.59	6
	ATOM	300	CG	GLN	A	301	21.644	31.003	50.808	1.00	40.26	6
	ATOM	301	CD	GLN	A	301	20.690	29.824	50.988	1.00	44.15	6
	ATOM	302	OE1	GLN	A	301	19.658	29.957	51.675	1.00	45.73	8
	ATOM	303	NE2	GLN	A	301	21.027	28.685	50.394	1.00	46.13	7
20	ATOM	304	C	GLN	A	301	21.242	34.305	48.877	1.00	41.64	6
	ATOM	305	O	GLN	A	301	21.482	34.185	47.686	1.00	45.02	8
	ATOM	306	N	ILE	A	302	20.413	35.228	49.372	1.00	41.01	7
	ATOM	307	CA	ILE	A	302	19.726	36.179	48.511	1.00	40.23	6
	ATOM	308	CB	ILE	A	302	18.502	36.774	49.217	1.00	39.52	6
25	ATOM	309	CG2	ILE	A	302	17.818	37.788	48.342	1.00	31.98	6
	ATOM	310	CG1	ILE	A	302	17.502	35.673	49.581	1.00	40.77	6
	ATOM	311	CD1	ILE	A	302	17.003	34.897	48.385	1.00	45.43	6
	ATOM	312	C	ILE	A	302	20.698	37.268	48.096	1.00	38.58	6
	ATOM	313	O	ILE	A	302	20.960	37.453	46.906	1.00	40.81	8
30	ATOM	314	N	ILE	A	303	21.228	37.972	49.097	1.00	37.50	7
	ATOM	315	CA	ILE	A	303	22.179	39.060	48.874	1.00	39.33	6
	ATOM	316	CB	ILE	A	303	23.023	39.338	50.109	1.00	39.06	6
	ATOM	317	CG2	ILE	A	303	23.946	40.522	49.861	1.00	36.19	6
	ATOM	318	CG1	ILE	A	303	22.141	39.653	51.313	1.00	40.15	6
35	ATOM	319	CD1	ILE	A	303	22.916	39.806	52.589	1.00	36.93	6
	ATOM	320	C	ILE	A	303	23.093	38.705	47.722	1.00	36.49	6
	ATOM	321	O	ILE	A	303	23.354	39.509	46.835	1.00	36.58	8
	ATOM	322	N	LEU	A	304	23.580	37.477	47.762	1.00	32.91	7
	ATOM	323	CA	LEU	A	304	24.465	36.964	46.734	1.00	27.55	6
40	ATOM	324	CB	LEU	A	304	24.935	35.554	47.123	1.00	22.35	6
	ATOM	325	CG	LEU	A	304	26.150	35.480	48.029	1.00	26.88	6
	ATOM	326	CD1	LEU	A	304	26.267	36.731	48.876	1.00	24.82	6
	ATOM	327	CD2	LEU	A	304	26.084	34.226	48.861	1.00	23.69	6
	ATOM	328	C	LEU	A	304	23.764	36.968	45.389	1.00	28.05	6
45	ATOM	329	O	LEU	A	304	24.212	37.623	44.443	1.00	24.68	8
	ATOM	330	N	LEU	A	305	22.657	36.236	45.318	1.00	26.34	7
	ATOM	331	CA	LEU	A	305	21.892	36.147	44.089	1.00	30.91	6
	ATOM	332	CB	LEU	A	305	20.565	35.434	44.359	1.00	32.50	6
	ATOM	333	CG	LEU	A	305	20.637	33.950	44.635	1.00	33.36	6
50	ATOM	334	CD1	LEU	A	305	19.247	33.370	44.779	1.00	33.87	6
	ATOM	335	CD2	LEU	A	305	21.340	33.280	43.466	1.00	31.72	6
	ATOM	336	C	LEU	A	305	21.665	37.524	43.477	1.00	29.76	6
	ATOM	337	O	LEU	A	305	21.954	37.747	42.301	1.00	29.33	8
	ATOM	338	N	LYS	A	306	21.157	38.439	44.298	1.00	29.72	7
55	ATOM	339	CA	LYS	A	306	20.868	39.800	43.864	1.00	34.28	6
	ATOM	340	CB	LYS	A	306	20.293	40.615	45.026	1.00	35.98	6
	ATOM	341	CG	LYS	A	306	18.919	40.163	45.511	1.00	43.35	6
	ATOM	342	CD	LYS	A	306	18.397	41.127	46.559	1.00	51.50	6

5	ATOM	343	CE	LYS	A	306	18.271	42.515	45.971	1.00	53.26	6
	ATOM	344	NZ	LYS	A	306	18.325	43.548	47.038	1.00	59.61	7
	ATOM	345	C	LYS	A	306	22.075	40.527	43.302	1.00	35.25	6
	ATOM	346	O	LYS	A	306	21.972	41.286	42.334	1.00	33.95	8
	ATOM	347	N	GLY	A	307	23.228	40.306	43.928	1.00	35.79	7
10	ATOM	348	CA	GLY	A	307	24.445	40.962	43.482	1.00	34.59	6
	ATOM	349	C	GLY	A	307	25.109	40.353	42.259	1.00	33.80	6
	ATOM	350	O	GLY	A	307	25.489	41.087	41.344	1.00	31.59	8
	ATOM	351	N	CYS	A	308	25.248	39.024	42.256	1.00	31.15	7
	ATOM	352	CA	CYS	A	308	25.899	38.326	41.174	1.00	29.04	6
15	ATOM	353	CB	CYS	A	308	26.604	37.089	41.704	1.00	27.59	6
	ATOM	354	SG	CYS	A	308	25.472	35.770	42.071	1.00	30.50	16
	ATOM	355	C	CYS	A	308	24.974	37.870	40.062	1.00	30.59	6
	ATOM	356	O	CYS	A	308	25.458	37.319	39.077	1.00	33.77	8
	ATOM	357	N	CYS	A	309	23.664	38.084	40.195	1.00	28.46	7
20	ATOM	358	CA	CYS	A	309	22.739	37.623	39.168	1.00	30.10	6
	ATOM	359	CB	CYS	A	309	21.311	38.004	39.490	1.00	33.43	6
	ATOM	360	SG	CYS	A	309	20.198	37.299	38.307	1.00	35.20	16
	ATOM	361	C	CYS	A	309	23.065	38.123	37.788	1.00	27.72	6
	ATOM	362	O	CYS	A	309	23.212	37.334	36.865	1.00	27.69	8
25	ATOM	363	N	MET	A	310	23.157	39.439	37.639	1.00	26.15	7
	ATOM	364	CA	MET	A	310	23.476	40.016	36.342	1.00	26.06	6
	ATOM	365	CB	MET	A	310	23.482	41.547	36.419	1.00	25.32	6
	ATOM	366	CG	MET	A	310	23.913	42.230	35.109	1.00	24.08	6
	ATOM	367	SD	MET	A	310	22.765	41.751	33.762	1.00	27.71	16
30	ATOM	368	CE	MET	A	310	23.650	42.321	32.270	1.00	28.50	6
	ATOM	369	C	MET	A	310	24.842	39.527	35.908	1.00	25.94	6
	ATOM	370	O	MET	A	310	25.020	39.076	34.788	1.00	28.09	8
	ATOM	371	N	GLU	A	311	25.800	39.638	36.826	1.00	25.39	7
	ATOM	372	CA	GLU	A	311	27.176	39.234	36.589	1.00	27.03	6
35	ATOM	373	CB	GLU	A	311	27.973	39.303	37.900	1.00	24.39	6
	ATOM	374	CG	GLU	A	311	27.842	40.628	38.668	1.00	26.00	6
	ATOM	375	CD	GLU	A	311	28.726	40.720	39.870	1.00	23.95	6
	ATOM	376	OE1	GLU	A	311	28.891	39.706	40.588	1.00	19.72	8
	ATOM	377	OE2	GLU	A	311	29.270	41.818	40.159	1.00	26.51	8
40	ATOM	378	C	GLU	A	311	27.266	37.827	35.997	1.00	27.51	6
	ATOM	379	O	GLU	A	311	27.956	37.620	35.014	1.00	29.67	8
	ATOM	380	N	ILE	A	312	26.569	36.866	36.602	1.00	26.82	7
	ATOM	381	CA	ILE	A	312	26.593	35.497	36.112	1.00	25.71	6
	ATOM	382	CB	ILE	A	312	25.991	34.518	37.123	1.00	23.35	6
45	ATOM	383	CG2	ILE	A	312	25.917	33.123	36.533	1.00	20.27	6
	ATOM	384	CG1	ILE	A	312	26.837	34.471	38.398	1.00	20.88	6
	ATOM	385	CD1	ILE	A	312	26.462	33.342	39.341	1.00	18.15	6
	ATOM	386	C	ILE	A	312	25.871	35.371	34.791	1.00	27.91	6
	ATOM	387	O	ILE	A	312	26.274	34.593	33.934	1.00	28.96	8
50	ATOM	388	N	MET	A	313	24.788	36.130	34.633	1.00	27.66	7
	ATOM	389	CA	MET	A	313	24.013	36.081	33.395	1.00	30.18	6
	ATOM	390	CB	MET	A	313	22.716	36.888	33.508	1.00	36.89	6
	ATOM	391	CG	MET	A	313	21.608	36.198	34.305	1.00	37.95	6
	ATOM	392	SD	MET	A	313	19.892	36.817	34.055	1.00	42.38	16
55	ATOM	393	CE	MET	A	313	20.034	38.503	34.740	1.00	40.68	6
	ATOM	394	C	MET	A	313	24.834	36.579	32.222	1.00	27.43	6
	ATOM	395	O	MET	A	313	25.116	35.814	31.308	1.00	28.61	8
	ATOM	396	N	SER	A	314	25.209	37.859	32.253	1.00	24.88	7

5	ATOM	397	CA	SER	A	314	26.005	38.472	31.197	1.00	27.98	6
	ATOM	398	CB	SER	A	314	26.354	39.914	31.581	1.00	29.64	6
	ATOM	399	OG	SER	A	314	26.956	39.972	32.858	1.00	43.44	8
	ATOM	400	C	SER	A	314	27.275	37.679	30.851	1.00	22.30	6
	ATOM	401	O	SER	A	314	27.675	37.629	29.690	1.00	24.18	8
10	ATOM	402	N	LEU	A	315	27.905	37.048	31.845	1.00	23.99	7
	ATOM	403	CA	LEU	A	315	29.099	36.261	31.563	1.00	25.07	6
	ATOM	404	CB	LEU	A	315	29.685	35.593	32.816	1.00	19.11	6
	ATOM	405	CG	LEU	A	315	30.675	34.479	32.505	1.00	20.39	6
	ATOM	406	CD1	LEU	A	315	31.866	35.040	31.756	1.00	18.92	6
15	ATOM	407	CD2	LEU	A	315	31.125	33.789	33.765	1.00	12.93	6
	ATOM	408	C	LEU	A	315	28.700	35.180	30.597	1.00	24.53	6
	ATOM	409	O	LEU	A	315	29.304	35.036	29.556	1.00	26.32	8
	ATOM	410	N	ARG	A	316	27.678	34.426	30.982	1.00	28.18	7
	ATOM	411	CA	ARG	A	316	27.151	33.312	30.216	1.00	27.54	6
20	ATOM	412	CB	ARG	A	316	25.915	32.752	30.928	1.00	27.39	6
	ATOM	413	CG	ARG	A	316	26.188	32.190	32.336	1.00	22.00	6
	ATOM	414	CD	ARG	A	316	24.934	31.526	32.901	1.00	18.78	6
	ATOM	415	NE	ARG	A	316	25.245	30.376	33.721	1.00	26.57	7
	ATOM	416	CZ	ARG	A	316	24.341	29.468	34.054	1.00	30.81	6
25	ATOM	417	NH1	ARG	A	316	23.084	29.614	33.639	1.00	33.71	7
	ATOM	418	NH2	ARG	A	316	24.701	28.416	34.776	1.00	33.13	7
	ATOM	419	C	ARG	A	316	26.774	33.660	28.794	1.00	28.09	6
	ATOM	420	O	ARG	A	316	26.737	32.792	27.931	1.00	32.41	8
	ATOM	421	N	ALA	A	317	26.484	34.936	28.571	1.00	28.36	7
30	ATOM	422	CA	ALA	A	317	26.094	35.411	27.264	1.00	26.64	6
	ATOM	423	CB	ALA	A	317	25.232	36.666	27.418	1.00	22.93	6
	ATOM	424	C	ALA	A	317	27.323	35.714	26.417	1.00	28.35	6
	ATOM	425	O	ALA	A	317	27.398	35.342	25.252	1.00	32.10	8
	ATOM	426	N	ALA	A	318	28.286	36.396	27.026	1.00	29.12	7
35	ATOM	427	CA	ALA	A	318	29.515	36.760	26.350	1.00	27.50	6
	ATOM	428	CB	ALA	A	318	30.434	37.452	27.333	1.00	28.39	6
	ATOM	429	C	ALA	A	318	30.181	35.502	25.825	1.00	28.10	6
	ATOM	430	O	ALA	A	318	30.600	35.447	24.678	1.00	28.18	8
	ATOM	431	N	VAL	A	319	30.255	34.491	26.700	1.00	29.16	7
40	ATOM	432	CA	VAL	A	319	30.880	33.198	26.393	1.00	35.24	6
	ATOM	433	CB	VAL	A	319	30.703	32.210	27.547	1.00	27.34	6
	ATOM	434	CG1	VAL	A	319	30.895	32.891	28.858	1.00	29.96	6
	ATOM	435	CG2	VAL	A	319	29.353	31.552	27.482	1.00	31.70	6
	ATOM	436	C	VAL	A	319	30.215	32.608	25.165	1.00	40.01	6
45	ATOM	437	O	VAL	A	319	30.640	31.575	24.680	1.00	42.70	8
	ATOM	438	N	ARG	A	320	29.176	33.284	24.683	1.00	38.64	7
	ATOM	439	CA	ARG	A	320	28.415	32.822	23.545	1.00	38.61	6
	ATOM	440	CB	ARG	A	320	27.031	32.458	24.043	1.00	37.26	6
	ATOM	441	CG	ARG	A	320	26.863	30.991	24.192	1.00	43.12	6
50	ATOM	442	CD	ARG	A	320	25.637	30.642	25.014	1.00	50.79	6
	ATOM	443	NE	ARG	A	320	25.258	29.256	24.770	1.00	54.71	7
	ATOM	444	CZ	ARG	A	320	24.331	28.625	25.501	1.00	57.89	6
	ATOM	445	NH1	ARG	A	320	23.667	29.291	26.440	1.00	49.08	7
	ATOM	446	NH2	ARG	A	320	23.964	27.385	25.242	1.00	59.59	7
55	ATOM	447	C	ARG	A	320	28.292	33.825	22.405	1.00	42.14	6
	ATOM	448	O	ARG	A	320	27.251	33.909	21.748	1.00	46.30	8
	ATOM	449	N	TYR	A	321	29.352	34.583	22.173	1.00	42.04	7
	ATOM	450	CA	TYR	A	321	29.366	35.555	21.098	1.00	42.70	6

5	ATOM	451	CB	TYR A 321	30.083	36.810	21.575	1.00	38.01	6
	ATOM	452	CG	TYR A 321	30.601	37.650	20.448	1.00	37.94	6
	ATOM	453	CD1	TYR A 321	29.733	38.296	19.574	1.00	33.85	6
	ATOM	454	CE1	TYR A 321	30.235	39.037	18.494	1.00	34.49	6
	ATOM	455	CD2	TYR A 321	31.966	37.743	20.224	1.00	28.03	6
10	ATOM	456	CE2	TYR A 321	32.473	38.475	19.153	1.00	32.69	6
	ATOM	457	CZ	TYR A 321	31.612	39.125	18.276	1.00	35.18	6
	ATOM	458	OH	TYR A 321	32.107	39.866	17.223	1.00	39.48	8
	ATOM	459	C	TYR A 321	30.085	35.005	19.877	1.00	45.51	6
	ATOM	460	O	TYR A 321	31.261	34.697	19.951	1.00	48.02	8
15	ATOM	461	N	ASP A 322	29.354	34.879	18.773	1.00	44.56	7
	ATOM	462	CA	ASP A 322	29.912	34.400	17.502	1.00	45.86	6
	ATOM	463	CB	ASP A 322	28.804	33.670	16.736	1.00	46.64	6
	ATOM	464	CG	ASP A 322	29.050	33.608	15.255	1.00	40.00	6
	ATOM	465	OD1	ASP A 322	30.010	34.256	14.768	1.00	40.00	8
20	ATOM	466	OD2	ASP A 322	28.262	32.929	14.536	1.00	40.00	8
	ATOM	467	C	ASP A 322	30.460	35.629	16.755	1.00	45.82	6
	ATOM	468	O	ASP A 322	29.678	36.464	16.271	1.00	45.38	8
	ATOM	469	N	PRO A 323	31.800	35.735	16.584	1.00	46.53	7
	ATOM	470	CD	PRO A 323	32.774	34.719	16.991	1.00	47.16	6
25	ATOM	471	CA	PRO A 323	32.424	36.889	15.890	1.00	46.63	6
	ATOM	472	CB	PRO A 323	33.921	36.603	15.936	1.00	43.95	6
	ATOM	473	CG	PRO A 323	34.099	35.303	16.582	1.00	43.93	6
	ATOM	474	C	PRO A 323	31.953	37.087	14.453	1.00	48.34	6
	ATOM	475	O	PRO A 323	31.797	38.210	13.960	1.00	50.84	8
30	ATOM	476	N	GLU A 324	31.778	35.970	13.752	1.00	52.39	7
	ATOM	477	CA	GLU A 324	31.339	35.968	12.370	1.00	55.85	6
	ATOM	478	CB	GLU A 324	31.035	34.528	11.965	1.00	55.54	6
	ATOM	479	CG	GLU A 324	32.224	33.584	12.104	1.00	40.00	6
	ATOM	480	CD	GLU A 324	33.432	34.023	11.310	1.00	40.00	6
35	ATOM	481	OE1	GLU A 324	33.350	35.040	10.555	1.00	40.00	8
	ATOM	482	OE2	GLU A 324	34.506	33.356	11.415	1.00	40.00	8
	ATOM	483	C	GLU A 324	30.077	36.798	12.277	1.00	54.94	6
	ATOM	484	O	GLU A 324	30.070	37.892	11.730	1.00	59.81	8
	ATOM	485	N	SER A 325	29.009	36.212	12.810	1.00	52.95	7
40	ATOM	486	CA	SER A 325	27.695	36.812	12.839	1.00	50.10	6
	ATOM	487	CB	SER A 325	26.701	35.797	13.402	1.00	48.23	6
	ATOM	488	OG	SER A 325	27.183	35.239	14.615	1.00	48.71	8
	ATOM	489	C	SER A 325	27.651	38.093	13.659	1.00	50.61	6
	ATOM	490	O	SER A 325	26.885	38.992	13.354	1.00	52.19	8
45	ATOM	491	N	GLU A 326	28.495	38.168	14.687	1.00	45.64	7
	ATOM	492	CA	GLU A 326	28.567	39.341	15.546	1.00	43.35	6
	ATOM	493	CB	GLU A 326	28.830	40.608	14.711	1.00	42.74	6
	ATOM	494	CG	GLU A 326	30.148	40.606	13.945	1.00	50.32	6
	ATOM	495	CD	GLU A 326	30.451	41.925	13.313	1.00	56.34	6
50	ATOM	496	OE1	GLU A 326	31.509	42.046	12.649	1.00	59.31	8
	ATOM	497	OE2	GLU A 326	29.656	42.890	13.452	1.00	55.74	8
	ATOM	498	C	GLU A 326	27.288	39.526	16.340	1.00	40.23	6
	ATOM	499	O	GLU A 326	26.695	40.603	16.340	1.00	40.44	8
	ATOM	500	N	THR A 327	26.888	38.474	17.051	1.00	35.90	7
55	ATOM	501	CA	THR A 327	25.663	38.506	17.860	1.00	37.29	6
	ATOM	502	CB	THR A 327	24.466	38.057	17.024	1.00	37.63	6
	ATOM	503	OG1	THR A 327	24.661	36.709	16.580	1.00	38.12	8
	ATOM	504	CG2	THR A 327	24.269	38.965	15.810	1.00	39.90	6

5	ATOM	505	C	THR A 327	25.767	37.562	19.038	1.00	39.49	6
	ATOM	506	O	THR A 327	26.284	36.458	18.903	1.00	40.50	8
	ATOM	507	N	LEU A 328	25.250	37.987	20.184	1.00	36.64	7
	ATOM	508	CA	LEU A 328	25.264	37.141	21.381	1.00	37.73	6
	ATOM	509	CB	LEU A 328	25.148	37.999	22.650	1.00	37.78	6
10	ATOM	510	CG	LEU A 328	26.102	39.150	22.843	1.00	36.26	6
	ATOM	511	CD1	LEU A 328	26.066	39.623	24.272	1.00	36.56	6
	ATOM	512	CD2	LEU A 328	27.481	38.688	22.500	1.00	39.85	6
	ATOM	513	C	LEU A 328	24.063	36.220	21.244	1.00	37.27	6
	ATOM	514	O	LEU A 328	23.306	36.337	20.279	1.00	34.96	8
15	ATOM	515	N	THR A 329	23.891	35.317	22.205	1.00	39.73	7
	ATOM	516	CA	THR A 329	22.785	34.376	22.180	1.00	40.81	6
	ATOM	517	CB	THR A 329	23.241	32.991	21.699	1.00	42.67	6
	ATOM	518	OG1	THR A 329	23.879	33.103	20.421	1.00	42.52	8
	ATOM	519	CG2	THR A 329	22.026	32.057	21.589	1.00	43.52	6
20	ATOM	520	C	THR A 329	22.168	34.245	23.548	1.00	44.31	6
	ATOM	521	O	THR A 329	22.526	33.370	24.320	1.00	43.72	8
	ATOM	522	N	LEU A 330	21.237	35.149	23.830	1.00	44.62	7
	ATOM	523	CA	LEU A 330	20.532	35.170	25.111	1.00	45.09	6
	ATOM	524	CB	LEU A 330	19.677	36.444	25.195	1.00	44.66	6
25	ATOM	525	CG	LEU A 330	20.436	37.750	25.259	1.00	51.06	6
	ATOM	526	CD1	LEU A 330	21.405	37.831	24.104	1.00	48.58	6
	ATOM	527	CD2	LEU A 330	19.466	38.909	25.238	1.00	45.18	6
	ATOM	528	C	LEU A 330	19.656	33.919	25.301	1.00	48.06	6
	ATOM	529	O	LEU A 330	19.049	33.422	24.359	1.00	49.33	8
30	ATOM	530	N	ASN A 331	19.618	33.431	26.540	1.00	52.20	7
	ATOM	531	CA	ASN A 331	18.842	32.256	26.913	1.00	54.41	6
	ATOM	532	CB	ASN A 331	17.361	32.628	27.009	1.00	54.94	6
	ATOM	533	CG	ASN A 331	16.724	32.112	28.269	1.00	60.35	6
	ATOM	534	OD1	ASN A 331	17.124	32.505	29.383	1.00	61.84	8
35	ATOM	535	ND2	ASN A 331	15.750	31.238	28.117	1.00	65.92	7
	ATOM	536	C	ASN A 331	19.016	31.108	25.934	1.00	58.00	6
	ATOM	537	O	ASN A 331	18.243	30.157	25.941	1.00	60.17	8
	ATOM	538	N	GLY A 332	20.063	31.196	25.114	1.00	58.45	7
	ATOM	539	CA	GLY A 332	20.341	30.161	24.131	1.00	58.55	6
40	ATOM	540	C	GLY A 332	19.316	30.016	23.021	1.00	59.79	6
	ATOM	541	O	GLY A 332	19.413	29.094	22.213	1.00	61.32	8
	ATOM	542	N	GLU A 333	18.346	30.929	22.983	1.00	60.28	7
	ATOM	543	CA	GLU A 333	17.294	30.883	21.985	1.00	59.13	6
	ATOM	544	CB	GLU A 333	15.919	30.875	22.662	1.00	62.40	6
45	ATOM	545	CG	GLU A 333	15.667	29.750	23.658	1.00	75.69	6
	ATOM	546	CD	GLU A 333	14.341	29.865	24.346	1.00	80.41	6
	ATOM	547	OE1	GLU A 333	14.052	30.932	24.945	1.00	79.98	8
	ATOM	548	OE2	GLU A 333	13.549	28.884	24.329	1.00	83.81	8
	ATOM	549	C	GLU A 333	17.356	32.090	21.073	1.00	57.18	6
50	ATOM	550	O	GLU A 333	17.239	31.969	19.852	1.00	57.50	8
	ATOM	551	N	MET A 334	17.512	33.258	21.696	1.00	55.20	7
	ATOM	552	CA	MET A 334	17.561	34.529	20.980	1.00	50.85	6
	ATOM	553	CB	MET A 334	16.751	35.556	21.763	1.00	48.70	6
	ATOM	554	CG	MET A 334	16.859	36.947	21.212	1.00	45.39	6
55	ATOM	555	SD	MET A 334	15.881	38.186	22.127	1.00	44.56	16
	ATOM	556	CE	MET A 334	14.229	37.371	22.113	1.00	45.25	6
	ATOM	557	C	MET A 334	18.956	35.087	20.713	1.00	51.59	6
	ATOM	558	O	MET A 334	19.739	35.268	21.633	1.00	52.52	8

5	ATOM	559	N	ALA	A	335	19.234	35.371	19.444	1.00	51.00	7
	ATOM	560	CA	ALA	A	335	20.520	35.932	19.039	1.00	48.98	6
	ATOM	561	CB	ALA	A	335	20.997	35.254	17.768	1.00	47.86	6
	ATOM	562	C	ALA	A	335	20.342	37.420	18.805	1.00	51.01	6
	ATOM	563	O	ALA	A	335	19.594	37.830	17.919	1.00	51.61	8
10	ATOM	564	N	VAL	A	336	21.024	38.232	19.612	1.00	46.62	7
	ATOM	565	CA	VAL	A	336	20.910	39.699	19.502	1.00	42.35	6
	ATOM	566	CB	VAL	A	336	20.517	40.325	20.840	1.00	42.41	6
	ATOM	567	CG1	VAL	A	336	19.242	39.691	21.361	1.00	42.00	6
	ATOM	568	CG2	VAL	A	336	21.639	40.211	21.852	1.00	40.32	6
15	ATOM	569	C	VAL	A	336	22.204	40.321	19.036	1.00	45.33	6
	ATOM	570	O	VAL	A	336	23.263	39.691	19.025	1.00	47.42	8
	ATOM	571	N	THR	A	337	22.090	41.590	18.668	1.00	41.60	7
	ATOM	572	CA	THR	A	337	23.230	42.377	18.175	1.00	39.69	6
	ATOM	573	CB	THR	A	337	22.882	43.061	16.852	1.00	41.35	6
20	ATOM	574	OG1	THR	A	337	21.987	44.157	17.080	1.00	49.35	8
	ATOM	575	CG2	THR	A	337	22.216	42.067	15.904	1.00	40.38	6
	ATOM	576	C	THR	A	337	23.588	43.481	19.159	1.00	37.88	6
	ATOM	577	O	THR	A	337	22.734	43.989	19.892	1.00	34.06	8
	ATOM	578	N	ARG	A	338	24.865	43.849	19.138	1.00	37.61	7
25	ATOM	579	CA	ARG	A	338	25.388	44.919	19.984	1.00	38.68	6
	ATOM	580	CB	ARG	A	338	26.669	45.479	19.351	1.00	35.95	6
	ATOM	581	CG	ARG	A	338	27.250	46.713	20.038	1.00	38.83	6
	ATOM	582	CD	ARG	A	338	28.443	47.254	19.247	1.00	35.88	6
	ATOM	583	NE	ARG	A	338	29.559	46.320	19.175	1.00	37.42	7
30	ATOM	584	CZ	ARG	A	338	30.449	46.122	20.145	1.00	30.20	6
	ATOM	585	NH1	ARG	A	338	30.338	46.791	21.295	1.00	27.98	7
	ATOM	586	NH2	ARG	A	338	31.433	45.240	19.954	1.00	27.40	7
	ATOM	587	C	ARG	A	338	24.333	46.010	20.085	1.00	38.09	6
	ATOM	588	O	ARG	A	338	23.894	46.397	21.169	1.00	34.12	8
35	ATOM	589	N	GLY	A	339	23.915	46.496	18.922	1.00	41.25	7
	ATOM	590	CA	GLY	A	339	22.918	47.547	18.890	1.00	41.35	6
	ATOM	591	C	GLY	A	339	21.692	47.140	19.672	1.00	41.23	6
	ATOM	592	O	GLY	A	339	21.445	47.671	20.750	1.00	38.30	8
	ATOM	593	N	GLN	A	340	20.924	46.203	19.105	1.00	38.58	7
40	ATOM	594	CA	GLN	A	340	19.701	45.700	19.729	1.00	40.79	6
	ATOM	595	CB	GLN	A	340	19.436	44.260	19.253	1.00	40.82	6
	ATOM	596	CG	GLN	A	340	19.087	44.146	17.767	1.00	41.10	6
	ATOM	597	CD	GLN	A	340	18.876	42.705	17.305	1.00	48.84	6
	ATOM	598	OE1	GLN	A	340	19.826	41.888	17.309	1.00	50.53	8
45	ATOM	599	NE2	GLN	A	340	17.650	42.393	16.907	1.00	54.25	7
	ATOM	600	C	GLN	A	340	19.779	45.750	21.263	1.00	41.50	6
	ATOM	601	O	GLN	A	340	18.998	46.444	21.923	1.00	42.72	8
	ATOM	602	N	LEU	A	341	20.758	45.026	21.806	1.00	42.00	7
	ATOM	603	CA	LEU	A	341	20.952	44.947	23.243	1.00	38.10	6
50	ATOM	604	CB	LEU	A	341	22.209	44.145	23.575	1.00	36.66	6
	ATOM	605	CG	LEU	A	341	22.361	43.804	25.029	1.00	39.94	6
	ATOM	606	CD1	LEU	A	341	21.219	42.884	25.410	1.00	34.98	6
	ATOM	607	CD2	LEU	A	341	23.685	43.128	25.284	1.00	40.95	6
	ATOM	608	C	LEU	A	341	21.072	46.321	23.860	1.00	36.37	6
55	ATOM	609	O	LEU	A	341	20.484	46.588	24.892	1.00	37.89	8
	ATOM	610	N	LYS	A	342	21.848	47.184	23.209	1.00	33.29	7
	ATOM	611	CA	LYS	A	342	22.089	48.546	23.679	1.00	35.17	6
	ATOM	612	CB	LYS	A	342	23.057	49.242	22.721	1.00	34.97	6



5	ATOM	613	CG	LYS	A	342	23.655	50.536	23.240	1.00	40.00	6
	ATOM	614	CD	LYS	A	342	24.673	51.109	22.245	1.00	34.48	6
	ATOM	615	CE	LYS	A	342	25.514	52.229	22.873	1.00	37.54	6
	ATOM	616	NZ	LYS	A	342	26.655	52.634	21.987	1.00	42.32	7
	ATOM	617	C	LYS	A	342	20.796	49.349	23.774	1.00	38.29	8
10	ATOM	618	O	LYS	A	342	20.345	49.711	24.861	1.00	36.23	8
	ATOM	619	N	ASN	A	343	20.223	49.622	22.603	1.00	39.25	7
	ATOM	620	CA	ASN	A	343	18.993	50.385	22.485	1.00	40.19	6
	ATOM	621	CB	ASN	A	343	18.521	50.373	21.033	1.00	37.96	6
	ATOM	622	CG	ASN	A	343	19.664	50.550	20.052	1.00	39.22	6
15	ATOM	623	OD1	ASN	A	343	20.428	51.537	20.125	1.00	42.37	8
	ATOM	624	ND2	ASN	A	343	19.773	49.612	19.125	1.00	42.19	7
	ATOM	625	C	ASN	A	343	17.928	49.748	23.375	1.00	40.12	6
	ATOM	626	O	ASN	A	343	17.010	50.417	23.859	1.00	36.01	8
	ATOM	627	N	GLY	A	344	18.073	48.433	23.568	1.00	40.95	7
20	ATOM	628	CA	GLY	A	344	17.152	47.670	24.394	1.00	39.25	6
	ATOM	629	C	GLY	A	344	17.039	48.092	25.842	1.00	38.26	6
	ATOM	630	O	GLY	A	344	16.072	47.724	26.512	1.00	35.69	8
	ATOM	631	N	GLY	A	345	18.017	48.857	26.329	1.00	35.89	7
	ATOM	632	CA	GLY	A	345	17.964	49.301	27.706	1.00	34.00	6
25	ATOM	633	C	GLY	A	345	19.273	49.199	28.443	1.00	38.64	6
	ATOM	634	O	GLY	A	345	19.469	49.888	29.441	1.00	38.14	8
	ATOM	635	N	LEU	A	346	20.170	48.337	27.973	1.00	39.52	7
	ATOM	636	CA	LEU	A	346	21.444	48.180	28.649	1.00	36.05	6
	ATOM	637	CB	LEU	A	346	22.124	46.876	28.209	1.00	35.72	6
30	ATOM	638	CG	LEU	A	346	21.355	45.617	28.501	1.00	34.89	6
	ATOM	639	CD1	LEU	A	346	22.295	44.413	28.422	1.00	44.09	6
	ATOM	640	CD2	LEU	A	346	20.786	45.721	29.902	1.00	34.84	6
	ATOM	641	C	LEU	A	346	22.358	49.361	28.396	1.00	33.52	6
	ATOM	642	O	LEU	A	346	23.267	49.653	29.178	1.00	35.58	8
35	ATOM	643	N	GLY	A	347	22.087	50.056	27.295	1.00	30.47	7
	ATOM	644	CA	GLY	A	347	22.909	51.192	26.931	1.00	33.01	6
	ATOM	645	C	GLY	A	347	24.360	50.768	26.747	1.00	30.72	6
	ATOM	646	O	GLY	A	347	24.669	49.775	26.082	1.00	30.89	8
	ATOM	647	N	VAL	A	348	25.244	51.556	27.355	1.00	31.30	7
40	ATOM	648	CA	VAL	A	348	26.671	51.325	27.286	1.00	31.27	6
	ATOM	649	CB	VAL	A	348	27.441	52.294	28.184	1.00	31.66	6
	ATOM	650	CG1	VAL	A	348	27.067	52.107	29.631	1.00	20.19	6
	ATOM	651	CG2	VAL	A	348	28.931	52.138	27.986	1.00	24.77	6
	ATOM	652	C	VAL	A	348	27.063	49.892	27.678	1.00	33.84	6
45	ATOM	653	O	VAL	A	348	28.095	49.392	27.225	1.00	29.99	8
	ATOM	654	N	VAL	A	349	26.253	49.227	28.514	1.00	33.31	7
	ATOM	655	CA	VAL	A	349	26.568	47.881	28.906	1.00	32.23	6
	ATOM	656	CB	VAL	A	349	25.581	47.259	29.858	1.00	32.59	6
	ATOM	657	CG1	VAL	A	349	25.865	45.795	29.985	1.00	33.68	6
50	ATOM	658	CG2	VAL	A	349	25.687	47.899	31.213	1.00	32.30	6
	ATOM	659	C	VAL	A	349	26.706	46.985	27.726	1.00	34.91	6
	ATOM	660	O	VAL	A	349	27.583	46.136	27.735	1.00	33.73	8
	ATOM	661	N	SER	A	350	25.875	47.134	26.702	1.00	32.81	7
	ATOM	662	CA	SER	A	350	26.001	46.252	25.556	1.00	30.10	6
55	ATOM	663	CB	SER	A	350	25.119	46.665	24.411	1.00	24.95	6
	ATOM	664	OG	SER	A	350	25.209	45.675	23.394	1.00	23.16	8
	ATOM	665	C	SER	A	350	27.445	46.257	25.129	1.00	31.59	6
	ATOM	666	O	SER	A	350	28.116	45.244	25.284	1.00	37.62	8

5	ATOM	667	N	ASP	A	351	27.945	47.367	24.591	1.00	28.60	7
	ATOM	668	CA	ASP	A	351	29.351	47.437	24.183	1.00	29.82	6
	ATOM	669	CB	ASP	A	351	29.808	48.891	24.105	1.00	27.49	6
	ATOM	670	CG	ASP	A	351	28.875	49.744	23.303	1.00	30.22	6
	ATOM	671	OD1	ASP	A	351	28.055	50.483	23.909	1.00	32.61	8
10	ATOM	672	OD2	ASP	A	351	28.942	49.714	22.044	1.00	30.02	8
	ATOM	673	C	ASP	A	351	30.173	46.653	25.231	1.00	30.63	6
	ATOM	674	O	ASP	A	351	30.981	45.792	24.903	1.00	29.54	8
	ATOM	675	N	ALA	A	352	29.939	46.949	26.503	1.00	25.33	7
	ATOM	676	CA	ALA	A	352	30.623	46.280	27.602	1.00	28.59	6
15	ATOM	677	CB	ALA	A	352	30.072	46.799	28.922	1.00	20.95	6
	ATOM	678	C	ALA	A	352	30.492	44.756	27.527	1.00	29.69	6
	ATOM	679	O	ALA	A	352	31.481	44.054	27.587	1.00	30.36	8
	ATOM	680	N	ILE	A	353	29.260	44.260	27.413	1.00	27.63	7
	ATOM	681	CA	ILE	A	353	29.003	42.832	27.326	1.00	27.55	6
20	ATOM	682	CB	ILE	A	353	27.512	42.528	27.429	1.00	28.04	6
	ATOM	683	CG2	ILE	A	353	27.269	41.042	27.289	1.00	23.68	6
	ATOM	684	CG1	ILE	A	353	26.955	42.965	28.789	1.00	27.33	6
	ATOM	685	CD1	ILE	A	353	25.452	42.688	28.944	1.00	26.23	6
	ATOM	686	C	ILE	A	353	29.534	42.207	26.054	1.00	30.88	6
25	ATOM	687	O	ILE	A	353	30.007	41.076	26.068	1.00	31.22	8
	ATOM	688	N	PHE	A	354	29.426	42.917	24.939	1.00	29.86	7
	ATOM	689	CA	PHE	A	354	29.922	42.369	23.686	1.00	31.08	6
	ATOM	690	CB	PHE	A	354	29.371	43.146	22.487	1.00	28.80	6
	ATOM	691	CG	PHE	A	354	28.029	42.643	21.988	1.00	28.80	6
30	ATOM	692	CD1	PHE	A	354	26.872	42.842	22.724	1.00	30.96	6
	ATOM	693	CD2	PHE	A	354	27.950	41.953	20.783	1.00	29.45	6
	ATOM	694	CE1	PHE	A	354	25.657	42.360	22.250	1.00	27.12	6
	ATOM	695	CE2	PHE	A	354	26.738	41.470	20.305	1.00	25.19	6
	ATOM	696	CZ	PHE	A	354	25.590	41.672	21.038	1.00	28.09	6
35	ATOM	697	C	PHE	A	354	31.444	42.399	23.682	1.00	29.17	6
	ATOM	698	O	PHE	A	354	32.087	41.389	23.398	1.00	32.62	8
	ATOM	699	N	ASP	A	355	32.013	43.569	23.980	1.00	23.86	7
	ATOM	700	CA	ASP	A	355	33.466	43.739	24.030	1.00	25.34	6
	ATOM	701	CB	ASP	A	355	33.820	45.053	24.737	1.00	21.41	6
40	ATOM	702	CG	ASP	A	355	33.841	46.226	23.809	1.00	32.08	6
	ATOM	703	OD1	ASP	A	355	32.979	46.322	22.902	1.00	33.58	8
	ATOM	704	OD2	ASP	A	355	34.711	47.117	23.968	1.00	33.20	8
	ATOM	705	C	ASP	A	355	34.074	42.559	24.781	1.00	27.86	6
	ATOM	706	O	ASP	A	355	35.131	42.053	24.410	1.00	32.42	8
45	ATOM	707	N	LEU	A	356	33.387	42.128	25.843	1.00	26.84	7
	ATOM	708	CA	LEU	A	356	33.845	40.993	26.642	1.00	28.66	6
	ATOM	709	CB	LEU	A	356	32.893	40.747	27.825	1.00	25.37	6
	ATOM	710	CG	LEU	A	356	33.235	39.608	28.755	1.00	27.61	6
	ATOM	711	CD1	LEU	A	356	34.538	39.917	29.451	1.00	25.43	6
50	ATOM	712	CD2	LEU	A	356	32.149	39.414	29.765	1.00	27.49	6
	ATOM	713	C	LEU	A	356	33.849	39.779	25.723	1.00	30.44	6
	ATOM	714	O	LEU	A	356	34.884	39.160	25.470	1.00	31.55	8
	ATOM	715	N	GLY	A	357	32.661	39.451	25.218	1.00	32.69	7
	ATOM	716	CA	GLY	A	357	32.511	38.304	24.338	1.00	29.87	6
55	ATOM	717	C	GLY	A	357	33.653	38.157	23.359	1.00	33.12	6
	ATOM	718	O	GLY	A	357	34.302	37.110	23.323	1.00	29.41	8
	ATOM	719	N	MET	A	358	33.876	39.206	22.564	1.00	33.31	7
	ATOM	720	CA	MET	A	358	34.949	39.206	21.580	1.00	35.87	6

5	ATOM	721	CB	MET	A	358	35.143	40.606	21.009	1.00	34.56	6
	ATOM	722	CG	MET	A	358	33.949	41.145	20.290	1.00	46.43	6
	ATOM	723	SD	MET	A	358	34.207	42.776	19.514	1.00	42.13	16
	ATOM	724	CE	MET	A	358	34.507	43.855	20.994	1.00	44.29	6
	ATOM	725	C	MET	A	358	36.256	38.762	22.230	1.00	33.26	6
10	ATOM	726	O	MET	A	358	36.894	37.807	21.795	1.00	36.39	8
	ATOM	727	N	SER	A	359	36.637	39.491	23.281	1.00	33.31	7
	ATOM	728	CA	SER	A	359	37.860	39.226	24.019	1.00	34.39	6
	ATOM	729	CB	SER	A	359	37.869	40.067	25.295	1.00	30.84	6
	ATOM	730	OG	SER	A	359	39.135	40.008	25.930	1.00	47.14	8
15	ATOM	731	C	SER	A	359	37.984	37.748	24.357	1.00	36.43	6
	ATOM	732	O	SER	A	359	38.900	37.078	23.896	1.00	35.46	8
	ATOM	733	N	LEU	A	360	37.046	37.264	25.166	1.00	36.74	7
	ATOM	734	CA	LEU	A	360	37.017	35.875	25.604	1.00	35.44	6
	ATOM	735	CB	LEU	A	360	35.708	35.579	26.336	1.00	34.16	6
20	ATOM	736	CG	LEU	A	360	35.471	36.290	27.644	1.00	34.59	6
	ATOM	737	CD1	LEU	A	360	34.225	35.765	28.312	1.00	33.53	6
	ATOM	738	CD2	LEU	A	360	36.658	36.052	28.541	1.00	31.69	6
	ATOM	739	C	LEU	A	360	37.203	34.862	24.500	1.00	38.72	6
	ATOM	740	O	LEU	A	360	37.820	33.828	24.728	1.00	38.29	8
25	ATOM	741	N	SER	A	361	36.635	35.147	23.328	1.00	40.96	7
	ATOM	742	CA	SER	A	361	36.777	34.262	22.186	1.00	45.67	6
	ATOM	743	CB	SER	A	361	36.518	35.045	20.904	1.00	46.45	6
	ATOM	744	OG	SER	A	361	35.210	35.598	20.906	1.00	51.81	8
	ATOM	745	C	SER	A	361	38.166	33.627	22.145	1.00	44.49	6
30	ATOM	746	O	SER	A	361	38.347	32.538	21.625	1.00	46.67	8
	ATOM	747	N	SER	A	362	39.134	34.348	22.703	1.00	41.44	7
	ATOM	748	CA	SER	A	362	40.525	33.918	22.790	1.00	42.13	6
	ATOM	749	CB	SER	A	362	41.408	35.131	23.066	1.00	42.61	6
	ATOM	750	OG	SER	A	362	41.219	36.136	22.076	1.00	51.87	8
35	ATOM	751	C	SER	A	362	40.798	32.870	23.876	1.00	38.41	6
	ATOM	752	O	SER	A	362	41.553	31.938	23.641	1.00	38.01	8
	ATOM	753	N	PHE	A	363	40.198	33.039	25.058	1.00	34.55	7
	ATOM	754	CA	PHE	A	363	40.417	32.126	26.174	1.00	32.96	6
	ATOM	755	CB	PHE	A	363	39.832	32.718	27.447	1.00	31.99	6
40	ATOM	756	CG	PHE	A	363	40.448	34.036	27.840	1.00	29.97	6
	ATOM	757	CD1	PHE	A	363	40.102	34.650	29.020	1.00	30.61	6
	ATOM	758	CD2	PHE	A	363	41.379	34.646	27.014	1.00	32.02	6
	ATOM	759	CE1	PHE	A	363	40.685	35.856	29.391	1.00	33.67	6
	ATOM	760	CE2	PHE	A	363	41.959	35.843	27.377	1.00	30.91	6
45	ATOM	761	CZ	PHE	A	363	41.615	36.456	28.558	1.00	29.33	6
	ATOM	762	C	PHE	A	363	39.883	30.716	25.967	1.00	30.52	6
	ATOM	763	O	PHE	A	363	40.436	29.766	26.526	1.00	32.19	8
	ATOM	764	N	ASN	A	364	38.817	30.570	25.175	1.00	33.51	7
	ATOM	765	CA	ASN	A	364	38.239	29.264	24.918	1.00	38.03	6
50	ATOM	766	CB	ASN	A	364	39.240	28.404	24.139	1.00	42.32	6
	ATOM	767	CG	ASN	A	364	39.696	29.065	22.861	1.00	53.11	6
	ATOM	768	OD1	ASN	A	364	38.874	29.330	21.954	1.00	59.51	8
	ATOM	769	ND2	ASN	A	364	40.986	29.330	22.772	1.00	55.95	7
	ATOM	770	C	ASN	A	364	37.916	28.572	26.235	1.00	31.89	6
55	ATOM	771	O	ASN	A	364	38.324	27.428	26.457	1.00	30.28	8
	ATOM	772	N	LEU	A	365	37.176	29.271	27.094	1.00	27.62	7
	ATOM	773	CA	LEU	A	365	36.806	28.743	28.406	1.00	29.36	6
	ATOM	774	CB	LEU	A	365	36.195	29.866	29.237	1.00	27.54	6

5	ATOM	775	CG	LEU	A	365	36.990	31.150	29.185	1.00	38.91	6
	ATOM	776	CD1	LEU	A	365	36.316	32.216	30.036	1.00	34.47	6
	ATOM	777	CD2	LEU	A	365	38.406	30.883	29.663	1.00	34.24	6
	ATOM	778	C	LEU	A	365	35.830	27.590	28.262	1.00	26.23	6
	ATOM	779	O	LEU	A	365	34.890	27.649	27.472	1.00	27.06	8
10	ATOM	780	N	ASP	A	366	36.083	26.528	29.021	1.00	25.23	7
	ATOM	781	CA	ASP	A	366	35.213	25.358	28.988	1.00	26.07	6
	ATOM	782	CB	ASP	A	366	36.027	24.049	29.033	1.00	29.68	6
	ATOM	783	CG	ASP	A	366	36.799	23.874	30.303	1.00	35.74	6
	ATOM	784	OD1	ASP	A	366	36.285	24.177	31.402	1.00	36.78	8
15	ATOM	785	OD2	ASP	A	366	37.959	23.386	30.240	1.00	41.23	8
	ATOM	786	C	ASP	A	366	34.278	25.434	30.181	1.00	27.70	6
	ATOM	787	O	ASP	A	366	34.587	26.097	31.173	1.00	31.94	8
	ATOM	788	N	ASP	A	367	33.141	24.743	30.066	1.00	29.18	7
	ATOM	789	CA	ASP	A	367	32.120	24.679	31.120	1.00	32.72	6
20	ATOM	790	CB	ASP	A	367	31.472	23.284	31.147	1.00	38.04	6
	ATOM	791	CG	ASP	A	367	30.806	22.924	29.854	1.00	42.43	6
	ATOM	792	OD1	ASP	A	367	29.877	23.650	29.409	1.00	35.95	8
	ATOM	793	OD2	ASP	A	367	31.186	21.884	29.250	1.00	51.42	8
	ATOM	794	C	ASP	A	367	32.754	24.969	32.482	1.00	33.71	6
25	ATOM	795	O	ASP	A	367	32.484	26.000	33.098	1.00	38.30	8
	ATOM	796	N	THR	A	368	33.602	24.032	32.919	1.00	31.06	7
	ATOM	797	CA	THR	A	368	34.329	24.124	34.181	1.00	26.28	6
	ATOM	798	CB	THR	A	368	35.559	23.222	34.141	1.00	27.30	6
	ATOM	799	OG1	THR	A	368	35.161	21.871	33.885	1.00	33.42	8
30	ATOM	800	CG2	THR	A	368	36.323	23.303	35.454	1.00	25.16	6
	ATOM	801	C	THR	A	368	34.764	25.557	34.479	1.00	21.13	6
	ATOM	802	O	THR	A	368	34.408	26.153	35.503	1.00	23.17	8
	ATOM	803	N	GLU	A	369	35.545	26.092	33.551	1.00	21.32	7
	ATOM	804	CA	GLU	A	369	36.065	27.435	33.661	1.00	28.00	6
35	ATOM	805	CB	GLU	A	369	36.960	27.707	32.453	1.00	32.79	6
	ATOM	806	CG	GLU	A	369	38.089	26.663	32.346	1.00	36.29	6
	ATOM	807	CD	GLU	A	369	38.906	26.747	31.110	1.00	41.03	6
	ATOM	808	OE1	GLU	A	369	38.337	26.744	29.994	1.00	42.05	8
	ATOM	809	OE2	GLU	A	369	40.158	26.795	31.218	1.00	42.03	8
40	ATOM	810	C	GLU	A	369	34.953	28.471	33.821	1.00	25.57	6
	ATOM	811	O	GLU	A	369	34.987	29.256	34.760	1.00	20.56	8
	ATOM	812	N	VAL	A	370	33.967	28.463	32.921	1.00	25.39	7
	ATOM	813	CA	VAL	A	370	32.849	29.396	33.029	1.00	25.99	6
	ATOM	814	CB	VAL	A	370	31.763	29.131	31.987	1.00	26.15	6
45	ATOM	815	CG1	VAL	A	370	30.609	30.093	32.183	1.00	27.65	6
	ATOM	816	CG2	VAL	A	370	32.306	29.251	30.592	1.00	17.70	6
	ATOM	817	C	VAL	A	370	32.245	29.209	34.412	1.00	26.49	6
	ATOM	818	O	VAL	A	370	32.012	30.170	35.147	1.00	28.16	8
	ATOM	819	N	ALA	A	371	31.988	27.947	34.739	1.00	21.01	7
50	ATOM	820	CA	ALA	A	371	31.393	27.554	36.011	1.00	19.57	6
	ATOM	821	CB	ALA	A	371	31.441	26.039	36.145	1.00	18.62	6
	ATOM	822	C	ALA	A	371	32.116	28.211	37.177	1.00	23.48	6
	ATOM	823	O	ALA	A	371	31.531	28.989	37.931	1.00	32.67	8
	ATOM	824	N	LEU	A	372	33.401	27.893	37.305	1.00	22.89	7
55	ATOM	825	CA	LEU	A	372	34.217	28.447	38.369	1.00	23.28	6
	ATOM	826	CB	LEU	A	372	35.675	27.996	38.178	1.00	27.76	6
	ATOM	827	CG	LEU	A	372	35.943	26.524	38.415	1.00	21.18	6
	ATOM	828	CD1	LEU	A	372	37.356	26.171	38.049	1.00	27.64	6

5	ATOM	829	CD2	LEU	A	372	35.675	26.204	39.880	1.00	20.90	6
	ATOM	830	C	LEU	A	372	34.098	29.966	38.396	1.00	21.34	6
	ATOM	831	O	LEU	A	372	33.828	30.572	39.439	1.00	23.16	8
	ATOM	832	N	LEU	A	373	34.288	30.561	37.223	1.00	24.42	7
	ATOM	833	CA	LEU	A	373	34.214	32.007	37.074	1.00	23.78	6
10	ATOM	834	CB	LEU	A	373	34.296	32.360	35.575	1.00	22.18	6
	ATOM	835	CG	LEU	A	373	34.784	33.726	35.165	1.00	31.52	6
	ATOM	836	CD1	LEU	A	373	36.000	34.084	35.962	1.00	31.93	6
	ATOM	837	CD2	LEU	A	373	35.103	33.720	33.693	1.00	30.24	6
	ATOM	838	C	LEU	A	373	32.904	32.480	37.720	1.00	25.69	6
15	ATOM	839	O	LEU	A	373	32.895	33.410	38.532	1.00	30.13	8
	ATOM	840	N	GLN	A	374	31.814	31.800	37.368	1.00	26.24	7
	ATOM	841	CA	GLN	A	374	30.487	32.104	37.896	1.00	21.60	6
	ATOM	842	CB	GLN	A	374	29.454	31.121	37.335	1.00	24.57	6
	ATOM	843	CG	GLN	A	374	29.310	31.145	35.821	1.00	21.02	6
20	ATOM	844	CD	GLN	A	374	28.224	30.201	35.331	1.00	22.86	6
	ATOM	845	OE1	GLN	A	374	28.037	30.042	34.123	1.00	24.07	8
	ATOM	846	NE2	GLN	A	374	27.515	29.590	36.249	1.00	25.59	7
	ATOM	847	C	GLN	A	374	30.421	32.039	39.422	1.00	20.66	6
	ATOM	848	O	GLN	A	374	29.717	32.832	40.048	1.00	24.47	8
25	ATOM	849	N	ALA	A	375	31.136	31.074	40.004	1.00	16.26	7
	ATOM	850	CA	ALA	A	375	31.155	30.889	41.445	1.00	17.16	6
	ATOM	851	CB	ALA	A	375	31.805	29.568	41.780	1.00	19.53	6
	ATOM	852	C	ALA	A	375	31.907	32.025	42.108	1.00	25.13	6
	ATOM	853	O	ALA	A	375	31.397	32.646	43.034	1.00	23.81	8
30	ATOM	854	N	VAL	A	376	33.122	32.277	41.611	1.00	24.57	7
	ATOM	855	CA	VAL	A	376	33.959	33.354	42.118	1.00	25.80	6
	ATOM	856	CB	VAL	A	376	35.101	33.658	41.164	1.00	26.48	6
	ATOM	857	CG1	VAL	A	376	35.926	34.812	41.697	1.00	23.20	6
	ATOM	858	CG2	VAL	A	376	35.959	32.429	40.952	1.00	19.08	6
35	ATOM	859	C	VAL	A	376	33.107	34.599	42.312	1.00	25.69	6
	ATOM	860	O	VAL	A	376	33.297	35.364	43.251	1.00	27.87	8
	ATOM	861	N	LEU	A	377	32.159	34.781	41.399	1.00	23.09	7
	ATOM	862	CA	LEU	A	377	31.242	35.915	41.423	1.00	22.86	6
	ATOM	863	CB	LEU	A	377	30.540	36.031	40.061	1.00	18.50	6
40	ATOM	864	CG	LEU	A	377	31.424	36.368	38.885	1.00	22.65	6
	ATOM	865	CD1	LEU	A	377	30.689	36.227	37.601	1.00	16.70	6
	ATOM	866	CD2	LEU	A	377	31.916	37.776	39.051	1.00	19.58	6
	ATOM	867	C	LEU	A	377	30.228	35.719	42.543	1.00	26.14	6
	ATOM	868	O	LEU	A	377	30.131	36.532	43.452	1.00	20.62	8
45	ATOM	869	N	LEU	A	378	29.483	34.614	42.468	1.00	28.99	7
	ATOM	870	CA	LEU	A	378	28.469	34.303	43.475	1.00	28.87	6
	ATOM	871	CB	LEU	A	378	28.053	32.826	43.397	1.00	26.89	6
	ATOM	872	CG	LEU	A	378	27.110	32.344	44.472	1.00	28.83	6
	ATOM	873	CD1	LEU	A	378	25.915	33.252	44.525	1.00	27.97	6
50	ATOM	874	CD2	LEU	A	378	26.693	30.928	44.205	1.00	27.69	6
	ATOM	875	C	LEU	A	378	28.992	34.617	44.853	1.00	31.09	6
	ATOM	876	O	LEU	A	378	28.399	35.421	45.573	1.00	31.77	8
	ATOM	877	N	MET	A	379	30.118	33.991	45.189	1.00	31.44	7
	ATOM	878	CA	MET	A	379	30.736	34.141	46.494	1.00	32.62	6
55	ATOM	879	CB	MET	A	379	31.690	32.960	46.744	1.00	31.45	6
	ATOM	880	CG	MET	A	379	30.984	31.595	46.792	1.00	38.75	6
	ATOM	881	SD	MET	A	379	29.741	31.626	48.107	1.00	41.27	16
	ATOM	882	CE	MET	A	379	28.896	30.036	47.851	1.00	35.68	6

5	ATOM	883	C	MET A 379	31.485	35.448	46.727	1.00	33.72	6
	ATOM	884	O	MET A 379	32.567	35.450	47.305	1.00	36.29	8
	ATOM	885	N	SER A 380	30.889	36.555	46.315	1.00	34.49	7
	ATOM	886	CA	SER A 380	31.498	37.853	46.550	1.00	33.97	6
	ATOM	887	CB	SER A 380	30.921	38.890	45.576	1.00	31.24	6
10	ATOM	888	OG	SER A 380	31.205	38.543	44.230	1.00	39.42	8
	ATOM	889	C	SER A 380	31.179	38.239	47.992	1.00	39.69	6
	ATOM	890	O	SER A 380	30.029	38.446	48.357	1.00	44.64	8
	ATOM	891	N	SER A 381	32.214	38.313	48.812	1.00	41.04	7
	ATOM	892	CA	SER A 381	32.060	38.640	50.216	1.00	44.91	6
15	ATOM	893	CB	SER A 381	33.324	38.234	50.951	1.00	44.50	6
	ATOM	894	OG	SER A 381	34.431	39.002	50.510	1.00	45.42	8
	ATOM	895	C	SER A 381	31.795	40.106	50.499	1.00	44.59	6
	ATOM	896	O	SER A 381	31.476	40.470	51.618	1.00	49.32	8
	ATOM	897	N	ASP A 382	31.939	40.942	49.486	1.00	43.75	7
20	ATOM	898	CA	ASP A 382	31.744	42.362	49.641	1.00	43.93	6
	ATOM	899	CB	ASP A 382	32.673	43.111	48.677	1.00	48.39	6
	ATOM	900	CG	ASP A 382	32.572	42.624	47.263	1.00	53.23	6
	ATOM	901	OD1	ASP A 382	32.705	41.400	47.034	1.00	56.97	8
	ATOM	902	OD2	ASP A 382	32.358	43.454	46.333	1.00	58.91	8
25	ATOM	903	C	ASP A 382	30.314	42.885	49.507	1.00	41.09	6
	ATOM	904	O	ASP A 382	30.048	44.036	49.845	1.00	40.93	8
	ATOM	905	N	ARG A 383	29.397	42.049	49.034	1.00	42.63	7
	ATOM	906	CA	ARG A 383	28.036	42.485	48.876	1.00	43.32	6
	ATOM	907	CB	ARG A 383	27.138	41.332	48.443	1.00	42.31	6
30	ATOM	908	CG	ARG A 383	27.651	40.399	47.352	1.00	40.83	6
	ATOM	909	CD	ARG A 383	27.586	40.954	45.925	1.00	38.09	6
	ATOM	910	NE	ARG A 383	27.768	39.878	44.975	1.00	37.33	7
	ATOM	911	CZ	ARG A 383	28.037	40.058	43.693	1.00	38.35	6
	ATOM	912	NH1	ARG A 383	28.142	41.292	43.198	1.00	33.70	7
35	ATOM	913	NH2	ARG A 383	28.194	38.992	42.918	1.00	35.46	7
	ATOM	914	C	ARG A 383	27.523	42.989	50.216	1.00	44.96	6
	ATOM	915	O	ARG A 383	27.744	42.344	51.260	1.00	45.60	8
	ATOM	916	N	PRO A 384	26.852	44.144	50.223	1.00	45.33	7
	ATOM	917	CD	PRO A 384	26.625	44.964	49.027	1.00	46.85	6
40	ATOM	918	CA	PRO A 384	26.298	44.738	51.446	1.00	47.37	6
	ATOM	919	CB	PRO A 384	25.841	46.130	51.012	1.00	46.90	6
	ATOM	920	CG	PRO A 384	26.075	46.229	49.567	1.00	46.41	6
	ATOM	921	C	PRO A 384	25.158	43.919	52.049	1.00	48.29	6
	ATOM	922	O	PRO A 384	24.404	43.264	51.329	1.00	48.34	8
45	ATOM	923	N	GLY A 385	25.039	43.983	53.383	1.00	49.88	7
	ATOM	924	CA	GLY A 385	23.991	43.270	54.113	1.00	50.35	6
	ATOM	925	C	GLY A 385	24.347	41.852	54.495	1.00	50.70	6
	ATOM	926	O	GLY A 385	23.614	41.204	55.244	1.00	53.48	8
	ATOM	927	N	LEU A 386	25.466	41.371	53.955	1.00	49.04	7
50	ATOM	928	CA	LEU A 386	25.901	40.017	54.215	1.00	50.53	6
	ATOM	929	CB	LEU A 386	27.224	39.751	53.492	1.00	45.17	6
	ATOM	930	CG	LEU A 386	27.152	39.592	51.993	1.00	48.26	6
	ATOM	931	CD1	LEU A 386	28.542	39.439	51.404	1.00	41.68	6
	ATOM	932	CD2	LEU A 386	26.302	38.374	51.682	1.00	38.40	6
55	ATOM	933	C	LEU A 386	26.045	39.776	55.691	1.00	52.13	6
	ATOM	934	O	LEU A 386	26.296	40.692	56.459	1.00	53.67	8
	ATOM	935	N	ALA A 387	25.861	38.522	56.077	1.00	53.42	7
	ATOM	936	CA	ALA A 387	25.976	38.129	57.470	1.00	56.01	6

5	ATOM	937	CB	ALA	A	387	24.802	37.234	57.854	1.00	56.47	6
	ATOM	938	C	ALA	A	387	27.289	37.385	57.659	1.00	55.52	6
	ATOM	939	O	ALA	A	387	28.275	37.940	58.134	1.00	53.75	8
	ATOM	940	N	CYS	A	388	27.273	36.120	57.253	1.00	56.03	7
	ATOM	941	CA	CYS	A	388	28.412	35.236	57.370	1.00	59.57	6
10	ATOM	942	CB	CYS	A	388	27.923	33.803	57.172	1.00	59.23	6
	ATOM	943	SG	CYS	A	388	26.397	33.431	58.009	1.00	58.64	16
	ATOM	944	C	CYS	A	388	29.482	35.581	56.328	1.00	62.18	6
	ATOM	945	O	CYS	A	388	29.720	34.821	55.400	1.00	67.88	8
	ATOM	946	N	VAL	A	389	30.110	36.747	56.495	1.00	60.78	7
15	ATOM	947	CA	VAL	A	389	31.173	37.212	55.590	1.00	57.70	6
	ATOM	948	CB	VAL	A	389	31.740	38.567	56.024	1.00	57.09	6
	ATOM	949	CG1	VAL	A	389	32.795	39.037	55.041	1.00	59.03	6
	ATOM	950	CG2	VAL	A	389	30.640	39.598	56.171	1.00	53.98	6
	ATOM	951	C	VAL	A	389	32.297	36.182	55.550	1.00	57.77	6
20	ATOM	952	O	VAL	A	389	32.358	35.336	54.662	1.00	60.94	8
	ATOM	953	N	ALA	A	390	33.182	36.292	56.528	1.00	52.68	7
	ATOM	954	CA	ALA	A	390	34.347	35.431	56.684	1.00	48.41	6
	ATOM	955	CB	ALA	A	390	34.703	35.321	58.185	1.00	45.19	6
	ATOM	956	C	ALA	A	390	34.224	34.040	56.082	1.00	47.63	6
25	ATOM	957	O	ALA	A	390	35.107	33.597	55.348	1.00	51.95	8
	ATOM	958	N	ARG	A	391	33.117	33.366	56.391	1.00	47.11	7
	ATOM	959	CA	ARG	A	391	32.879	32.018	55.885	1.00	51.64	6
	ATOM	960	CB	ARG	A	391	31.520	31.498	56.383	1.00	54.22	6
	ATOM	961	CG	ARG	A	391	31.267	30.012	56.059	1.00	64.20	6
30	ATOM	962	CD	ARG	A	391	29.930	29.489	56.602	1.00	73.80	6
	ATOM	963	NE	ARG	A	391	29.787	28.044	56.454	1.00	79.76	7
	ATOM	964	CZ	ARG	A	391	30.573	27.140	57.043	1.00	84.27	6
	ATOM	965	NH1	ARG	A	391	31.598	27.535	57.806	1.00	85.28	7
	ATOM	966	NH2	ARG	A	391	30.340	25.840	56.849	1.00	86.84	7
35	ATOM	967	C	ARG	A	391	32.922	31.986	54.358	1.00	48.18	6
	ATOM	968	O	ARG	A	391	33.494	31.080	53.756	1.00	49.57	8
	ATOM	969	N	ILE	A	392	32.281	32.993	53.762	1.00	45.01	7
	ATOM	970	CA	ILE	A	392	32.196	33.148	52.319	1.00	48.77	6
	ATOM	971	CB	ILE	A	392	31.224	34.297	51.963	1.00	46.45	6
40	ATOM	972	CG2	ILE	A	392	31.241	34.582	50.479	1.00	42.35	6
	ATOM	973	CG1	ILE	A	392	29.791	33.953	52.402	1.00	49.69	6
	ATOM	974	CD1	ILE	A	392	28.792	35.039	52.113	1.00	51.09	6
	ATOM	975	C	ILE	A	392	33.554	33.356	51.641	1.00	50.90	6
	ATOM	976	O	ILE	A	392	33.914	32.605	50.732	1.00	52.21	8
45	ATOM	977	N	GLU	A	393	34.298	34.374	52.071	1.00	50.43	7
	ATOM	978	CA	GLU	A	393	35.592	34.684	51.471	1.00	50.30	6
	ATOM	979	CB	GLU	A	393	36.437	35.561	52.387	1.00	53.97	6
	ATOM	980	CG	GLU	A	393	36.558	36.966	51.844	1.00	62.18	6
	ATOM	981	CD	GLU	A	393	37.546	37.777	52.564	1.00	67.69	6
50	ATOM	982	OE1	GLU	A	393	38.149	38.741	52.119	1.00	66.42	8
	ATOM	983	OE2	GLU	A	393	37.856	37.640	53.729	1.00	70.64	8
	ATOM	984	C	GLU	A	393	36.341	33.429	51.230	1.00	49.31	6
	ATOM	985	O	GLU	A	393	36.755	33.089	50.125	1.00	49.53	8
	ATOM	986	N	LYS	A	394	36.552	32.730	52.303	1.00	46.07	7
55	ATOM	987	CA	LYS	A	394	37.265	31.543	52.078	1.00	45.76	6
	ATOM	988	CB	LYS	A	394	37.396	30.800	53.373	1.00	43.85	6
	ATOM	989	CG	LYS	A	394	38.207	31.617	54.394	1.00	40.00	6
	ATOM	990	CD	LYS	A	394	39.372	32.374	53.705	1.00	40.00	6

5	ATOM	991	CE	LYS	A	394	40.136	33.265	54.681	1.00	40.00	6
	ATOM	992	NZ	LYS	A	394	41.516	33.602	54.162	1.00	40.00	7
	ATOM	993	C	LYS	A	394	36.568	30.778	50.966	1.00	46.69	6
	ATOM	994	O	LYS	A	394	37.215	30.427	49.988	1.00	49.13	8
	ATOM	995	N	TYR	A	395	35.269	30.514	51.095	1.00	46.57	7
10	ATOM	996	CA	TYR	A	395	34.553	29.823	50.022	1.00	43.33	6
	ATOM	997	CB	TYR	A	395	33.059	30.123	50.076	1.00	48.44	6
	ATOM	998	CG	TYR	A	395	32.275	29.236	50.994	1.00	53.83	6
	ATOM	999	CD1	TYR	A	395	31.010	29.598	51.415	1.00	56.43	6
	ATOM	1000	CE1	TYR	A	395	30.266	28.769	52.252	1.00	59.73	6
15	ATOM	1001	CD2	TYR	A	395	32.790	28.033	51.428	1.00	56.47	6
	ATOM	1002	CE2	TYR	A	395	32.054	27.198	52.265	1.00	62.60	6
	ATOM	1003	CZ	TYR	A	395	30.787	27.565	52.687	1.00	63.18	6
	ATOM	1004	OH	TYR	A	395	30.059	26.753	53.528	1.00	64.46	8
	ATOM	1005	C	TYR	A	395	35.120	30.356	48.716	1.00	37.30	6
20	ATOM	1006	O	TYR	A	395	35.643	29.601	47.908	1.00	34.10	8
	ATOM	1007	N	GLN	A	396	35.029	31.670	48.522	1.00	31.92	7
	ATOM	1008	CA	GLN	A	396	35.563	32.273	47.305	1.00	34.81	6
	ATOM	1009	CB	GLN	A	396	35.403	33.801	47.329	1.00	32.64	6
	ATOM	1010	CG	GLN	A	396	36.088	34.485	46.162	1.00	29.57	6
25	ATOM	1011	CD	GLN	A	396	35.616	35.891	45.927	1.00	29.46	6
	ATOM	1012	OE1	GLN	A	396	35.599	36.726	46.862	1.00	34.65	8
	ATOM	1013	NE2	GLN	A	396	35.245	36.173	44.689	1.00	27.21	7
	ATOM	1014	C	GLN	A	396	37.035	31.909	47.167	1.00	37.13	6
	ATOM	1015	O	GLN	A	396	37.511	31.590	46.080	1.00	37.36	8
30	ATOM	1016	N	ASP	A	397	37.751	31.970	48.285	1.00	38.61	7
	ATOM	1017	CA	ASP	A	397	39.164	31.642	48.298	1.00	40.37	6
	ATOM	1018	CB	ASP	A	397	39.757	31.869	49.704	1.00	40.51	6
	ATOM	1019	CG	ASP	A	397	39.813	33.319	50.095	1.00	43.77	6
	ATOM	1020	OD1	ASP	A	397	40.397	34.123	49.334	1.00	46.50	8
35	ATOM	1021	OD2	ASP	A	397	39.299	33.702	51.184	1.00	51.34	8
	ATOM	1022	C	ASP	A	397	39.302	30.176	47.898	1.00	38.62	6
	ATOM	1023	O	ASP	A	397	40.230	29.809	47.199	1.00	39.20	8
	ATOM	1024	N	SER	A	398	38.350	29.359	48.344	1.00	37.84	7
	ATOM	1025	CA	SER	A	398	38.348	27.929	48.063	1.00	37.80	6
40	ATOM	1026	CB	SER	A	398	37.240	27.240	48.878	1.00	34.28	6
	ATOM	1027	OG	SER	A	398	37.297	25.826	48.755	1.00	46.60	8
	ATOM	1028	C	SER	A	398	38.164	27.639	46.581	1.00	38.41	6
	ATOM	1029	O	SER	A	398	38.677	26.642	46.075	1.00	39.98	8
	ATOM	1030	N	PHE	A	399	37.419	28.507	45.893	1.00	34.82	7
45	ATOM	1031	CA	PHE	A	399	37.181	28.325	44.462	1.00	35.96	6
	ATOM	1032	CB	PHE	A	399	35.873	28.983	44.015	1.00	35.75	6
	ATOM	1033	CG	PHE	A	399	34.632	28.216	44.403	1.00	39.30	6
	ATOM	1034	CD1	PHE	A	399	34.107	28.294	45.677	1.00	39.86	6
	ATOM	1035	CD2	PHE	A	399	34.018	27.393	43.488	1.00	36.81	6
50	ATOM	1036	CE1	PHE	A	399	32.961	27.557	46.013	1.00	41.25	6
	ATOM	1037	CE2	PHE	A	399	32.880	26.661	43.825	1.00	43.61	6
	ATOM	1038	CZ	PHE	A	399	32.354	26.740	45.087	1.00	40.34	6
	ATOM	1039	C	PHE	A	399	38.328	28.890	43.630	1.00	33.48	6
	ATOM	1040	O	PHE	A	399	38.867	28.200	42.756	1.00	26.86	8
55	ATOM	1041	N	LEU	A	400	38.680	30.156	43.877	1.00	31.47	7
	ATOM	1042	CA	LEU	A	400	39.754	30.796	43.132	1.00	37.41	6
	ATOM	1043	CB	LEU	A	400	40.179	32.100	43.814	1.00	34.24	6
	ATOM	1044	CG	LEU	A	400	39.239	33.265	43.628	1.00	35.10	6



5	ATOM	1045	CD1	LEU	A	400	39.803	34.531	44.256	1.00	26.60	6
	ATOM	1046	CD2	LEU	A	400	39.065	33.479	42.137	1.00	29.44	6
	ATOM	1047	C	LEU	A	400	40.941	29.872	42.947	1.00	38.84	6
	ATOM	1048	O	LEU	A	400	41.367	29.632	41.821	1.00	40.38	8
	ATOM	1049	N	LEU	A	401	41.464	29.350	44.055	1.00	42.79	7
10	ATOM	1050	CA	LEU	A	401	42.605	28.449	43.988	1.00	43.48	6
	ATOM	1051	CB	LEU	A	401	42.900	27.821	45.355	1.00	44.73	6
	ATOM	1052	CG	LEU	A	401	44.105	26.899	45.354	1.00	51.39	6
	ATOM	1053	CD1	LEU	A	401	45.374	27.749	45.143	1.00	50.11	6
	ATOM	1054	CD2	LEU	A	401	44.205	26.122	46.662	1.00	49.30	6
15	ATOM	1055	C	LEU	A	401	42.324	27.340	42.981	1.00	41.62	6
	ATOM	1056	O	LEU	A	401	43.052	27.180	42.004	1.00	45.14	8
	ATOM	1057	N	ALA	A	402	41.269	26.574	43.245	1.00	37.92	7
	ATOM	1058	CA	ALA	A	402	40.873	25.469	42.386	1.00	29.90	6
	ATOM	1059	CB	ALA	A	402	39.522	24.928	42.834	1.00	30.70	6
20	ATOM	1060	C	ALA	A	402	40.798	25.909	40.929	1.00	28.88	6
	ATOM	1061	O	ALA	A	402	41.277	25.203	40.034	1.00	32.14	8
	ATOM	1062	N	PHE	A	403	40.200	27.086	40.707	1.00	31.07	7
	ATOM	1063	CA	PHE	A	403	40.052	27.642	39.363	1.00	29.90	6
	ATOM	1064	CB	PHE	A	403	39.379	29.019	39.438	1.00	27.03	6
25	ATOM	1065	CG	PHE	A	403	38.943	29.574	38.100	1.00	26.97	6
	ATOM	1066	CD1	PHE	A	403	38.228	30.758	38.033	1.00	25.55	6
	ATOM	1067	CD2	PHE	A	403	39.224	28.905	36.925	1.00	19.75	6
	ATOM	1068	CE1	PHE	A	403	37.784	31.266	36.808	1.00	27.90	6
	ATOM	1069	CE2	PHE	A	403	38.780	29.416	35.694	1.00	22.56	6
30	ATOM	1070	CZ	PHE	A	403	38.063	30.596	35.640	1.00	22.24	6
	ATOM	1071	C	PHE	A	403	41.429	27.756	38.719	1.00	28.82	6
	ATOM	1072	O	PHE	A	403	41.666	27.210	37.646	1.00	26.00	8
	ATOM	1073	N	GLU	A	404	42.329	28.463	39.402	1.00	30.25	7
	ATOM	1074	CA	GLU	A	404	43.695	28.665	38.922	1.00	34.03	6
35	ATOM	1075	CB	GLU	A	404	44.513	29.416	39.983	1.00	39.45	6
	ATOM	1076	CG	GLU	A	404	45.867	29.935	39.489	1.00	47.68	6
	ATOM	1077	CD	GLU	A	404	46.734	30.507	40.571	1.00	54.02	6
	ATOM	1078	OE1	GLU	A	404	46.236	31.298	41.408	1.00	57.27	8
	ATOM	1079	OE2	GLU	A	404	47.956	30.202	40.606	1.00	63.85	8
40	ATOM	1080	C	GLU	A	404	44.352	27.322	38.634	1.00	36.01	6
	ATOM	1081	O	GLU	A	404	44.936	27.112	37.574	1.00	38.64	8
	ATOM	1082	N	HIS	A	405	44.259	26.420	39.610	1.00	29.56	7
	ATOM	1083	CA	HIS	A	405	44.840	25.093	39.468	1.00	31.69	6
	ATOM	1084	CB	HIS	A	405	44.540	24.228	40.694	1.00	33.75	6
45	ATOM	1085	CG	HIS	A	405	45.292	24.657	41.908	1.00	34.75	6
	ATOM	1086	CD2	HIS	A	405	46.198	25.640	42.130	1.00	34.58	6
	ATOM	1087	ND1	HIS	A	405	45.161	23.984	43.130	1.00	32.43	7
	ATOM	1088	CE1	HIS	A	405	45.975	24.568	44.018	1.00	36.15	6
	ATOM	1089	NE2	HIS	A	405	46.601	25.561	43.430	1.00	39.84	7
50	ATOM	1090	C	HIS	A	405	44.274	24.445	38.225	1.00	34.21	6
	ATOM	1091	O	HIS	A	405	45.029	23.949	37.386	1.00	37.06	8
	ATOM	1092	N	TYR	A	406	42.947	24.453	38.100	1.00	30.83	7
	ATOM	1093	CA	TYR	A	406	42.313	23.859	36.930	1.00	28.85	6
	ATOM	1094	CB	TYR	A	406	40.805	24.080	36.934	1.00	31.48	6
55	ATOM	1095	CG	TYR	A	406	40.139	23.494	35.709	1.00	23.49	6
	ATOM	1096	CD1	TYR	A	406	40.073	22.123	35.532	1.00	19.42	6
	ATOM	1097	CE1	TYR	A	406	39.517	21.577	34.382	1.00	23.80	6
	ATOM	1098	CD2	TYR	A	406	39.646	24.313	34.704	1.00	21.81	6

5	ATOM	1099	CE2	TYR	A	406	39.090	23.769	33.551	1.00	24.64	6
	ATOM	1100	CZ	TYR	A	406	39.029	22.395	33.380	1.00	21.56	6
	ATOM	1101	OH	TYR	A	406	38.489	21.850	32.236	1.00	24.96	8
	ATOM	1102	C	TYR	A	406	42.882	24.504	35.672	1.00	24.24	6
	ATOM	1103	O	TYR	A	406	42.958	23.872	34.621	1.00	27.08	8
10	ATOM	1104	N	ILE	A	407	43.253	25.784	35.807	1.00	25.76	7
	ATOM	1105	CA	ILE	A	407	43.824	26.548	34.705	1.00	33.75	6
	ATOM	1106	CB	ILE	A	407	43.986	28.033	35.070	1.00	34.23	6
	ATOM	1107	CG2	ILE	A	407	44.967	28.712	34.139	1.00	32.46	6
	ATOM	1108	CG1	ILE	A	407	42.615	28.728	35.042	1.00	43.30	6
15	ATOM	1109	CD1	ILE	A	407	41.896	28.602	33.694	1.00	40.40	6
	ATOM	1110	C	ILE	A	407	45.143	25.973	34.256	1.00	39.03	6
	ATOM	1111	O	ILE	A	407	45.383	25.771	33.063	1.00	35.18	8
	ATOM	1112	N	ASN	A	408	46.003	25.721	35.227	1.00	37.25	7
	ATOM	1113	CA	ASN	A	408	47.307	25.194	34.926	1.00	37.01	6
20	ATOM	1114	CB	ASN	A	408	48.107	25.017	36.213	1.00	32.27	6
	ATOM	1115	CG	ASN	A	408	48.346	26.362	36.936	1.00	33.56	6
	ATOM	1116	OD1	ASN	A	408	48.827	27.335	36.320	1.00	31.99	8
	ATOM	1117	ND2	ASN	A	408	48.038	26.403	38.231	1.00	31.23	7
	ATOM	1118	C	ASN	A	408	47.205	23.892	34.136	1.00	38.14	6
25	ATOM	1119	O	ASN	A	408	47.900	23.734	33.124	1.00	42.16	8
	ATOM	1120	N	TYR	A	409	46.334	22.981	34.568	1.00	35.62	7
	ATOM	1121	CA	TYR	A	409	46.159	21.710	33.866	1.00	35.91	6
	ATOM	1122	CB	TYR	A	409	45.051	20.859	34.507	1.00	34.41	6
	ATOM	1123	CG	TYR	A	409	44.624	19.687	33.619	1.00	38.73	6
30	ATOM	1124	CD1	TYR	A	409	45.563	18.765	33.155	1.00	41.34	6
	ATOM	1125	CE1	TYR	A	409	45.186	17.709	32.321	1.00	47.16	6
	ATOM	1126	CD2	TYR	A	409	43.292	19.515	33.232	1.00	46.20	6
	ATOM	1127	CE2	TYR	A	409	42.913	18.455	32.397	1.00	50.74	6
	ATOM	1128	CZ	TYR	A	409	43.863	17.551	31.946	1.00	50.88	6
35	ATOM	1129	OH	TYR	A	409	43.498	16.514	31.130	1.00	53.14	8
	ATOM	1130	C	TYR	A	409	45.760	21.966	32.424	1.00	38.16	6
	ATOM	1131	O	TYR	A	409	46.202	21.281	31.502	1.00	41.83	8
	ATOM	1132	N	ARG	A	410	44.872	22.943	32.272	1.00	42.25	7
	ATOM	1133	CA	ARG	A	410	44.345	23.332	30.984	1.00	42.83	6
40	ATOM	1134	CB	ARG	A	410	43.311	24.427	31.195	1.00	36.83	6
	ATOM	1135	CG	ARG	A	410	41.994	23.979	31.795	1.00	34.32	6
	ATOM	1136	CD	ARG	A	410	41.073	23.504	30.675	1.00	36.62	6
	ATOM	1137	NE	ARG	A	410	40.888	24.550	29.685	1.00	38.64	7
	ATOM	1138	CZ	ARG	A	410	40.177	24.397	28.576	1.00	35.73	6
45	ATOM	1139	NH1	ARG	A	410	39.572	23.230	28.348	1.00	33.17	7
	ATOM	1140	NH2	ARG	A	410	40.077	25.407	27.708	1.00	32.70	7
	ATOM	1141	C	ARG	A	410	45.442	23.850	30.083	1.00	46.67	6
	ATOM	1142	O	ARG	A	410	45.467	23.591	28.882	1.00	41.78	8
	ATOM	1143	N	LYS	A	411	46.360	24.577	30.710	1.00	52.99	7
50	ATOM	1144	CA	LYS	A	411	47.467	25.194	30.017	1.00	58.32	6
	ATOM	1145	CB	LYS	A	411	48.645	24.216	29.876	1.00	64.99	6
	ATOM	1146	CG	LYS	A	411	48.349	22.835	29.367	1.00	70.48	6
	ATOM	1147	CD	LYS	A	411	49.608	21.974	29.494	1.00	77.18	6
	ATOM	1148	CE	LYS	A	411	49.461	20.621	28.795	1.00	84.30	6
55	ATOM	1149	NZ	LYS	A	411	50.740	19.828	28.857	1.00	86.48	7
	ATOM	1150	C	LYS	A	411	47.032	25.756	28.686	1.00	56.66	6
	ATOM	1151	O	LYS	A	411	47.160	25.153	27.633	1.00	55.47	8
	ATOM	1152	N	HIS	A	412	46.458	26.943	28.823	1.00	54.67	7

5	ATOM	1153	CA	HIS	A	412	45.984	27.722	27.705	1.00	48.67	6
	ATOM	1154	CB	HIS	A	412	45.124	28.884	28.201	1.00	43.14	6
	ATOM	1155	CG	HIS	A	412	43.812	28.480	28.755	1.00	41.36	6
	ATOM	1156	CD2	HIS	A	412	43.429	28.064	29.987	1.00	35.44	6
	ATOM	1157	ND1	HIS	A	412	42.651	28.440	27.966	1.00	38.19	7
10	ATOM	1158	CE1	HIS	A	412	41.648	28.014	28.723	1.00	34.75	6
	ATOM	1159	NE2	HIS	A	412	42.094	27.780	29.942	1.00	35.52	7
	ATOM	1160	C	HIS	A	412	47.231	28.303	27.101	1.00	46.35	6
	ATOM	1161	O	HIS	A	412	48.269	28.452	27.775	1.00	42.73	8
	ATOM	1162	N	HIS	A	413	47.116	28.696	25.839	1.00	48.92	7
15	ATOM	1163	CA	HIS	A	413	48.234	29.290	25.146	1.00	53.15	6
	ATOM	1164	CB	HIS	A	413	48.404	28.666	23.755	1.00	55.27	6
	ATOM	1165	CG	HIS	A	413	49.326	29.446	22.886	1.00	58.77	6
	ATOM	1166	CD2	HIS	A	413	49.213	30.660	22.304	1.00	61.65	6
	ATOM	1167	ND1	HIS	A	413	50.617	28.997	22.564	1.00	60.31	7
20	ATOM	1168	CE1	HIS	A	413	51.214	29.924	21.828	1.00	63.01	6
	ATOM	1169	NE2	HIS	A	413	50.386	30.941	21.658	1.00	62.93	7
	ATOM	1170	C	HIS	A	413	47.932	30.768	24.998	1.00	53.19	6
	ATOM	1171	O	HIS	A	413	47.639	31.301	23.934	1.00	54.93	8
	ATOM	1172	N	VAL	A	414	47.964	31.413	26.139	1.00	53.77	7
25	ATOM	1173	CA	VAL	A	414	47.735	32.811	26.146	1.00	51.06	6
	ATOM	1174	CB	VAL	A	414	46.291	33.183	26.417	1.00	51.49	6
	ATOM	1175	CG1	VAL	A	414	46.186	34.715	26.603	1.00	45.22	6
	ATOM	1176	CG2	VAL	A	414	45.419	32.732	25.263	1.00	52.67	6
	ATOM	1177	C	VAL	A	414	48.623	33.283	27.226	1.00	54.28	6
30	ATOM	1178	O	VAL	A	414	48.427	33.029	28.409	1.00	55.49	8
	ATOM	1179	N	THR	A	415	49.706	33.863	26.733	1.00	56.28	7
	ATOM	1180	CA	THR	A	415	50.721	34.484	27.557	1.00	57.83	6
	ATOM	1181	CB	THR	A	415	51.268	35.675	26.758	1.00	59.64	6
	ATOM	1182	OG1	THR	A	415	51.605	36.754	27.636	1.00	66.69	8
35	ATOM	1183	CG2	THR	A	415	50.197	36.158	25.745	1.00	59.42	6
	ATOM	1184	C	THR	A	415	50.146	35.049	28.879	1.00	56.98	6
	ATOM	1185	O	THR	A	415	48.933	35.146	29.051	1.00	55.70	8
	ATOM	1186	N	HIS	A	416	51.068	35.330	29.795	1.00	57.44	7
	ATOM	1187	CA	HIS	A	416	50.808	36.011	31.047	1.00	57.34	6
40	ATOM	1188	CB	HIS	A	416	51.346	37.422	30.708	1.00	61.35	6
	ATOM	1189	CG	HIS	A	416	51.872	38.237	31.821	1.00	69.78	6
	ATOM	1190	CD2	HIS	A	416	53.114	38.297	32.390	1.00	71.42	6
	ATOM	1191	ND1	HIS	A	416	51.135	39.263	32.416	1.00	72.49	7
	ATOM	1192	CE1	HIS	A	416	51.914	39.884	33.290	1.00	75.50	6
45	ATOM	1193	NE2	HIS	A	416	53.099	39.323	33.291	1.00	73.91	7
	ATOM	1194	C	HIS	A	416	49.261	35.892	31.297	1.00	53.79	6
	ATOM	1195	O	HIS	A	416	48.499	36.779	30.902	1.00	52.81	8
	ATOM	1196	N	PHE	A	417	48.806	34.779	31.911	1.00	48.05	7
	ATOM	1197	CA	PHE	A	417	47.355	34.428	32.061	1.00	47.99	6
50	ATOM	1198	CB	PHE	A	417	47.165	32.954	31.996	1.00	46.11	6
	ATOM	1199	CG	PHE	A	417	45.835	32.590	31.399	1.00	44.27	6
	ATOM	1200	CD1	PHE	A	417	45.680	32.720	30.046	1.00	41.79	6
	ATOM	1201	CD2	PHE	A	417	44.758	32.135	32.164	1.00	40.23	6
	ATOM	1202	CE1	PHE	A	417	44.498	32.397	29.422	1.00	44.30	6
55	ATOM	1203	CE2	PHE	A	417	43.540	31.802	31.529	1.00	36.80	6
	ATOM	1204	CZ	PHE	A	417	43.427	31.928	30.144	1.00	40.69	6
	ATOM	1205	C	PHE	A	417	46.427	34.836	33.196	1.00	46.69	6
	ATOM	1206	O	PHE	A	417	46.147	36.004	33.331	1.00	43.35	8

5	ATOM	1207	N	TRP	A	418	45.906	33.801	33.909	1.00	45.14	7
	ATOM	1208	CA	TRP	A	418	44.982	33.867	35.065	1.00	44.89	6
	ATOM	1209	CB	TRP	A	418	45.545	33.099	36.255	1.00	42.24	6
	ATOM	1210	CG	TRP	A	418	44.959	33.452	37.598	1.00	47.11	6
	ATOM	1211	CD2	TRP	A	418	43.724	32.924	38.149	1.00	46.98	6
10	ATOM	1212	CE2	TRP	A	418	43.534	33.565	39.413	1.00	48.94	6
	ATOM	1213	CE3	TRP	A	418	42.777	31.986	37.688	1.00	45.23	6
	ATOM	1214	CD1	TRP	A	418	45.434	34.350	38.512	1.00	46.24	6
	ATOM	1215	NE1	TRP	A	418	44.588	34.407	39.608	1.00	50.63	7
	ATOM	1216	CZ2	TRP	A	418	42.441	33.270	40.238	1.00	45.46	6
15	ATOM	1217	CZ3	TRP	A	418	41.686	31.706	38.500	1.00	44.50	6
	ATOM	1218	CH2	TRP	A	418	41.511	32.335	39.753	1.00	47.55	6
	ATOM	1219	C	TRP	A	418	44.908	35.324	35.398	1.00	43.88	6
	ATOM	1220	O	TRP	A	418	43.797	35.839	35.702	1.00	43.17	8
	ATOM	1221	N	PRO	A	419	46.084	35.976	35.461	1.00	43.55	7
20	ATOM	1222	CD	PRO	A	419	47.467	35.482	35.400	1.00	41.52	6
	ATOM	1223	CA	PRO	A	419	46.009	37.396	35.758	1.00	41.48	6
	ATOM	1224	CB	PRO	A	419	47.436	37.884	35.535	1.00	39.21	6
	ATOM	1225	CG	PRO	A	419	48.261	36.696	35.223	1.00	39.25	6
	ATOM	1226	C	PRO	A	419	44.960	38.090	34.817	1.00	36.28	6
25	ATOM	1227	O	PRO	A	419	44.208	38.978	35.237	1.00	37.08	8
	ATOM	1228	N	LYS	A	420	44.915	37.701	33.540	1.00	35.96	7
	ATOM	1229	CA	LYS	A	420	43.977	38.287	32.575	1.00	40.82	6
	ATOM	1230	CB	LYS	A	420	44.314	37.805	31.155	1.00	40.78	6
	ATOM	1231	CG	LYS	A	420	45.684	38.244	30.641	1.00	48.62	6
30	ATOM	1232	CD	LYS	A	420	45.904	37.781	29.206	1.00	55.12	6
	ATOM	1233	CE	LYS	A	420	47.248	38.261	28.673	1.00	53.26	6
	ATOM	1234	NZ	LYS	A	420	47.448	37.884	27.222	1.00	52.69	7
	ATOM	1235	C	LYS	A	420	42.580	37.832	32.948	1.00	40.29	6
	ATOM	1236	O	LYS	A	420	41.656	38.626	32.982	1.00	39.66	8
35	ATOM	1237	N	LEU	A	421	42.461	36.537	33.245	1.00	38.33	7
	ATOM	1238	CA	LEU	A	421	41.186	35.931	33.613	1.00	37.60	6
	ATOM	1239	CB	LEU	A	421	41.397	34.433	33.915	1.00	43.66	6
	ATOM	1240	CG	LEU	A	421	40.204	33.518	33.828	1.00	46.50	6
	ATOM	1241	CD1	LEU	A	421	39.643	33.624	32.426	1.00	45.15	6
40	ATOM	1242	CD2	LEU	A	421	40.595	32.094	34.131	1.00	51.31	6
	ATOM	1243	C	LEU	A	421	40.575	36.664	34.808	1.00	39.59	6
	ATOM	1244	O	LEU	A	421	39.371	36.910	34.837	1.00	40.66	8
	ATOM	1245	N	LEU	A	422	41.412	37.017	35.782	1.00	39.57	7
	ATOM	1246	CA	LEU	A	422	40.946	37.726	36.961	1.00	38.63	6
45	ATOM	1247	CB	LEU	A	422	42.085	37.890	37.971	1.00	41.79	6
	ATOM	1248	CG	LEU	A	422	42.424	36.671	38.798	1.00	42.74	6
	ATOM	1249	CD1	LEU	A	422	43.490	37.010	39.820	1.00	42.89	6
	ATOM	1250	CD2	LEU	A	422	41.168	36.216	39.523	1.00	39.27	6
	ATOM	1251	C	LEU	A	422	40.381	39.073	36.589	1.00	40.47	6
50	ATOM	1252	O	LEU	A	422	39.428	39.525	37.210	1.00	47.83	8
	ATOM	1253	N	MET	A	423	40.969	39.698	35.569	1.00	34.27	7
	ATOM	1254	CA	MET	A	423	40.511	41.001	35.117	1.00	35.25	6
	ATOM	1255	CB	MET	A	423	41.427	41.553	34.028	1.00	32.56	6
	ATOM	1256	CG	MET	A	423	42.856	41.732	34.456	1.00	40.70	6
55	ATOM	1257	SD	MET	A	423	43.707	43.101	33.619	1.00	47.65	16
	ATOM	1258	CE	MET	A	423	43.348	42.776	31.848	1.00	47.16	6
	ATOM	1259	C	MET	A	423	39.100	40.899	34.574	1.00	35.13	6
	ATOM	1260	O	MET	A	423	38.315	41.829	34.696	1.00	29.85	8

5	ATOM	1261	N	LYS	A	424	38.791	39.752	33.975	1.00	31.56	7
	ATOM	1262	CA	LYS	A	424	37.470	39.529	33.423	1.00	32.29	6
	ATOM	1263	CB	LYS	A	424	37.446	38.205	32.658	1.00	30.56	6
	ATOM	1264	CG	LYS	A	424	38.394	38.192	31.455	1.00	30.07	6
	ATOM	1265	CD	LYS	A	424	38.050	39.326	30.488	1.00	33.22	6
10	ATOM	1266	CE	LYS	A	424	39.032	39.433	29.322	1.00	28.75	6
	ATOM	1267	NZ	LYS	A	424	40.394	39.942	29.707	1.00	31.01	7
	ATOM	1268	C	LYS	A	424	36.418	39.558	34.524	1.00	29.26	6
	ATOM	1269	O	LYS	A	424	35.307	39.998	34.289	1.00	30.22	8
	ATOM	1270	N	VAL	A	425	36.796	39.098	35.719	1.00	23.53	7
15	ATOM	1271	CA	VAL	A	425	35.897	39.107	36.866	1.00	28.91	6
	ATOM	1272	CB	VAL	A	425	36.541	38.460	38.094	1.00	29.44	6
	ATOM	1273	CG1	VAL	A	425	35.673	38.642	39.320	1.00	28.81	6
	ATOM	1274	CG2	VAL	A	425	36.764	36.985	37.849	1.00	31.22	6
	ATOM	1275	C	VAL	A	425	35.512	40.548	37.161	1.00	32.03	6
20	ATOM	1276	O	VAL	A	425	34.350	40.839	37.429	1.00	31.95	8
	ATOM	1277	N	THR	A	426	36.496	41.444	37.124	1.00	33.61	7
	ATOM	1278	CA	THR	A	426	36.248	42.866	37.356	1.00	30.76	6
	ATOM	1279	CB	THR	A	426	37.559	43.670	37.360	1.00	32.34	6
	ATOM	1280	OG1	THR	A	426	38.209	43.565	38.630	1.00	33.07	8
25	ATOM	1281	CG2	THR	A	426	37.302	45.131	37.015	1.00	25.40	6
	ATOM	1282	C	THR	A	426	35.363	43.324	36.211	1.00	32.53	6
	ATOM	1283	O	THR	A	426	34.357	44.006	36.405	1.00	35.19	8
	ATOM	1284	N	ASP	A	427	35.763	42.929	35.006	1.00	28.83	7
	ATOM	1285	CA	ASP	A	427	35.011	43.272	33.810	1.00	35.12	6
30	ATOM	1286	CB	ASP	A	427	35.556	42.524	32.578	1.00	39.14	6
	ATOM	1287	CG	ASP	A	427	36.837	43.103	32.057	1.00	45.80	6
	ATOM	1288	OD1	ASP	A	427	36.982	44.346	32.024	1.00	41.97	8
	ATOM	1289	OD2	ASP	A	427	37.735	42.333	31.616	1.00	50.06	8
	ATOM	1290	C	ASP	A	427	33.537	42.925	34.028	1.00	33.94	6
35	ATOM	1291	O	ASP	A	427	32.659	43.712	33.702	1.00	38.02	8
	ATOM	1292	N	LEU	A	428	33.283	41.745	34.584	1.00	27.15	7
	ATOM	1293	CA	LEU	A	428	31.925	41.293	34.850	1.00	29.99	6
	ATOM	1294	CB	LEU	A	428	31.924	39.786	35.133	1.00	22.49	6
	ATOM	1295	CG	LEU	A	428	32.104	38.873	33.939	1.00	25.54	6
40	ATOM	1296	CD1	LEU	A	428	32.202	37.421	34.353	1.00	20.60	6
	ATOM	1297	CD2	LEU	A	428	30.920	39.083	33.029	1.00	17.24	6
	ATOM	1298	C	LEU	A	428	31.276	42.057	35.991	1.00	28.94	6
	ATOM	1299	O	LEU	A	428	30.082	42.306	35.939	1.00	31.26	8
	ATOM	1300	N	ARG	A	429	32.059	42.423	37.011	1.00	27.64	7
45	ATOM	1301	CA	ARG	A	429	31.527	43.162	38.147	1.00	28.13	6
	ATOM	1302	CB	ARG	A	429	32.564	43.298	39.264	1.00	29.59	6
	ATOM	1303	CG	ARG	A	429	32.818	42.040	40.080	1.00	34.85	6
	ATOM	1304	CD	ARG	A	429	33.588	42.360	41.367	1.00	47.18	6
	ATOM	1305	NE	ARG	A	429	34.093	41.175	42.049	1.00	57.93	7
50	ATOM	1306	CZ	ARG	A	429	33.327	40.210	42.547	1.00	63.62	6
	ATOM	1307	NH1	ARG	A	429	31.998	40.270	42.396	1.00	60.71	7
	ATOM	1308	NH2	ARG	A	429	33.900	39.165	43.150	1.00	62.38	7
	ATOM	1309	C	ARG	A	429	31.099	44.536	37.707	1.00	29.81	6
	ATOM	1310	O	ARG	A	429	30.044	45.009	38.101	1.00	30.81	8
55	ATOM	1311	N	MET	A	430	31.941	45.176	36.901	1.00	29.64	7
	ATOM	1312	CA	MET	A	430	31.644	46.502	36.383	1.00	34.72	6
	ATOM	1313	CB	MET	A	430	32.745	46.955	35.434	1.00	34.97	6
	ATOM	1314	CG	MET	A	430	33.937	47.597	36.080	1.00	45.34	6

5	ATOM	1315	SD	MET	A	430	33.520	49.120	36.937	1.00	52.55	16
	ATOM	1316	CE	MET	A	430	32.942	50.174	35.585	1.00	55.56	6
	ATOM	1317	C	MET	A	430	30.315	46.455	35.634	1.00	34.01	6
	ATOM	1318	O	MET	A	430	29.455	47.295	35.854	1.00	37.29	8
	ATOM	1319	N	ILE	A	431	30.180	45.468	34.740	1.00	29.99	7
10	ATOM	1320	CA	ILE	A	431	28.954	45.269	33.969	1.00	28.82	6
	ATOM	1321	CB	ILE	A	431	28.962	43.936	33.211	1.00	27.39	6
	ATOM	1322	CG2	ILE	A	431	27.622	43.671	32.572	1.00	23.87	6
	ATOM	1323	CG1	ILE	A	431	30.044	43.920	32.138	1.00	25.56	6
	ATOM	1324	CD1	ILE	A	431	29.989	42.703	31.244	1.00	17.29	6
15	ATOM	1325	C	ILE	A	431	27.769	45.269	34.907	1.00	29.49	6
	ATOM	1326	O	ILE	A	431	26.810	45.993	34.712	1.00	24.19	8
	ATOM	1327	N	GLY	A	432	27.839	44.435	35.936	1.00	25.25	7
	ATOM	1328	CA	GLY	A	432	26.748	44.343	36.890	1.00	30.38	6
	ATOM	1329	C	GLY	A	432	26.494	45.671	37.554	1.00	32.75	6
20	ATOM	1330	O	GLY	A	432	25.411	46.206	37.469	1.00	36.38	8
	ATOM	1331	N	ALA	A	433	27.514	46.189	38.221	1.00	26.77	7
	ATOM	1332	CA	ALA	A	433	27.428	47.459	38.910	1.00	26.48	6
	ATOM	1333	CB	ALA	A	433	28.836	47.970	39.203	1.00	19.90	6
	ATOM	1334	C	ALA	A	433	26.663	48.502	38.114	1.00	30.73	6
25	ATOM	1335	O	ALA	A	433	25.773	49.164	38.635	1.00	31.60	8
	ATOM	1336	N	CYS	A	434	27.027	48.654	36.854	1.00	33.22	7
	ATOM	1337	CA	CYS	A	434	26.371	49.616	35.996	1.00	34.34	6
	ATOM	1338	CB	CYS	A	434	27.047	49.612	34.711	1.00	35.20	6
	ATOM	1339	SG	CYS	A	434	27.789	50.811	34.285	1.00	54.48	16
30	ATOM	1340	C	CYS	A	434	24.974	49.198	35.612	1.00	34.09	6
	ATOM	1341	O	CYS	A	434	24.107	50.040	35.415	1.00	34.89	8
	ATOM	1342	N	HIS	A	435	24.756	47.898	35.447	1.00	34.30	7
	ATOM	1343	CA	HIS	A	435	23.453	47.423	35.042	1.00	35.44	6
	ATOM	1344	CB	HIS	A	435	23.404	45.904	35.104	1.00	31.76	6
35	ATOM	1345	CG	HIS	A	435	22.099	45.351	34.675	1.00	32.03	6
	ATOM	1346	CD2	HIS	A	435	21.697	44.790	33.519	1.00	28.61	6
	ATOM	1347	ND1	HIS	A	435	20.941	45.482	35.452	1.00	28.48	7
	ATOM	1348	CE1	HIS	A	435	19.912	45.025	34.759	1.00	33.27	6
	ATOM	1349	NE2	HIS	A	435	20.345	44.597	33.583	1.00	31.57	7
40	ATOM	1350	C	HIS	A	435	22.400	47.974	35.972	1.00	32.74	6
	ATOM	1351	O	HIS	A	435	21.304	48.284	35.565	1.00	32.87	8
	ATOM	1352	N	ALA	A	436	22.777	48.046	37.241	1.00	31.01	7
	ATOM	1353	CA	ALA	A	436	21.910	48.563	38.266	1.00	29.91	6
	ATOM	1354	CB	ALA	A	436	22.661	48.595	39.580	1.00	21.23	6
45	ATOM	1355	C	ALA	A	436	21.475	49.969	37.884	1.00	33.86	6
	ATOM	1356	O	ALA	A	436	20.296	50.298	37.910	1.00	36.10	8
	ATOM	1357	N	SER	A	437	22.453	50.795	37.532	1.00	35.19	7
	ATOM	1358	CA	SER	A	437	22.172	52.167	37.140	1.00	33.03	6
	ATOM	1359	CB	SER	A	437	23.441	52.815	36.603	1.00	35.31	6
50	ATOM	1360	OG	SER	A	437	23.203	54.151	36.193	1.00	44.99	8
	ATOM	1361	C	SER	A	437	21.110	52.158	36.055	1.00	38.39	6
	ATOM	1362	O	SER	A	437	20.049	52.745	36.204	1.00	37.54	8
	ATOM	1363	N	ARG	A	438	21.432	51.483	34.956	1.00	37.32	7
	ATOM	1364	CA	ARG	A	438	20.534	51.379	33.821	1.00	39.30	6
55	ATOM	1365	CB	ARG	A	438	21.114	50.402	32.786	1.00	42.97	6
	ATOM	1366	CG	ARG	A	438	22.343	50.911	32.051	1.00	41.72	6
	ATOM	1367	CD	ARG	A	438	21.955	52.134	31.251	1.00	45.23	6
	ATOM	1368	NE	ARG	A	438	20.964	51.839	30.237	1.00	45.66	7

5	ATOM	1369	CZ	ARG	A	438	20.063	52.718	29.809	1.00	49.71	6
	ATOM	1370	NH1	ARG	A	438	20.046	53.958	30.318	1.00	50.91	7
	ATOM	1371	NH2	ARG	A	438	19.198	52.354	28.865	1.00	46.86	7
	ATOM	1372	C	ARG	A	438	19.147	50.922	34.240	1.00	42.37	6
	ATOM	1373	O	ARG	A	438	18.147	51.297	33.625	1.00	40.58	8
10	ATOM	1374	N	PHE	A	439	19.080	50.120	35.298	1.00	42.25	7
	ATOM	1375	CA	PHE	A	439	17.803	49.624	35.763	1.00	42.81	6
	ATOM	1376	CB	PHE	A	439	17.975	48.794	37.013	1.00	42.18	6
	ATOM	1377	CG	PHE	A	439	16.739	48.053	37.413	1.00	42.48	6
	ATOM	1378	CD1	PHE	A	439	16.198	47.111	36.562	1.00	47.09	6
15	ATOM	1379	CD2	PHE	A	439	16.105	48.320	38.613	1.00	39.76	6
	ATOM	1380	CE1	PHE	A	439	15.047	46.427	36.905	1.00	49.17	6
	ATOM	1381	CE2	PHE	A	439	14.940	47.630	38.963	1.00	45.10	6
	ATOM	1382	CZ	PHE	A	439	14.411	46.683	38.098	1.00	46.36	6
	ATOM	1383	C	PHE	A	439	16.921	50.803	36.075	1.00	44.79	6
20	ATOM	1384	O	PHE	A	439	15.830	50.903	35.554	1.00	40.26	8
	ATOM	1385	N	LEU	A	440	17.410	51.681	36.951	1.00	42.77	7
	ATOM	1386	CA	LEU	A	440	16.660	52.871	37.344	1.00	42.96	6
	ATOM	1387	CB	LEU	A	440	17.546	53.824	38.150	1.00	37.19	6
	ATOM	1388	CG	LEU	A	440	17.943	53.297	39.500	1.00	36.97	6
25	ATOM	1389	CD1	LEU	A	440	18.620	54.389	40.316	1.00	33.65	6
	ATOM	1390	CD2	LEU	A	440	16.679	52.837	40.216	1.00	35.42	6
	ATOM	1391	C	LEU	A	440	16.025	53.596	36.168	1.00	45.47	6
	ATOM	1392	O	LEU	A	440	14.809	53.750	36.126	1.00	52.48	8
	ATOM	1393	N	HIS	A	441	16.836	54.060	35.223	1.00	49.15	7
30	ATOM	1394	CA	HIS	A	441	16.277	54.725	34.063	1.00	54.76	6
	ATOM	1395	CB	HIS	A	441	17.329	54.955	33.031	1.00	56.68	6
	ATOM	1396	CG	HIS	A	441	18.134	56.161	33.282	1.00	62.73	6
	ATOM	1397	CD2	HIS	A	441	18.468	57.216	32.499	1.00	65.73	6
	ATOM	1398	ND1	HIS	A	441	18.701	56.431	34.538	1.00	66.01	7
35	ATOM	1399	CE1	HIS	A	441	19.332	57.594	34.473	1.00	65.55	6
	ATOM	1400	NE2	HIS	A	441	19.205	58.085	33.255	1.00	60.09	7
	ATOM	1401	C	HIS	A	441	15.244	53.822	33.481	1.00	55.93	6
	ATOM	1402	O	HIS	A	441	14.149	54.263	33.170	1.00	57.33	8
	ATOM	1403	N	MET	A	442	15.605	52.549	33.313	1.00	57.81	7
40	ATOM	1404	CA	MET	A	442	14.661	51.583	32.778	1.00	59.11	6
	ATOM	1405	CB	MET	A	442	15.191	50.154	32.922	1.00	55.93	6
	ATOM	1406	CG	MET	A	442	16.336	49.813	32.022	1.00	58.52	6
	ATOM	1407	SD	MET	A	442	16.681	48.008	31.851	1.00	60.99	16
	ATOM	1408	CE	MET	A	442	17.085	47.602	33.581	1.00	52.61	6
45	ATOM	1409	C	MET	A	442	13.339	51.727	33.534	1.00	60.31	6
	ATOM	1410	O	MET	A	442	12.266	51.560	32.968	1.00	58.18	8
	ATOM	1411	N	LYS	A	443	13.425	52.054	34.818	1.00	61.45	7
	ATOM	1412	CA	LYS	A	443	12.236	52.202	35.626	1.00	64.90	6
	ATOM	1413	CB	LYS	A	443	12.608	52.141	37.090	1.00	64.40	6
50	ATOM	1414	CG	LYS	A	443	11.461	51.748	37.959	1.00	69.12	6
	ATOM	1415	CD	LYS	A	443	12.068	51.551	39.257	1.00	71.14	6
	ATOM	1416	CE	LYS	A	443	11.368	51.897	40.091	1.00	73.43	6
	ATOM	1417	NZ	LYS	A	443	11.883	51.712	41.415	1.00	67.97	7
	ATOM	1418	C	LYS	A	443	11.513	53.514	35.348	1.00	67.29	6
55	ATOM	1419	O	LYS	A	443	10.390	53.700	35.780	1.00	67.90	8
	ATOM	1420	N	VAL	A	444	12.171	54.429	34.629	1.00	66.57	7
	ATOM	1421	CA	VAL	A	444	11.575	55.719	34.297	1.00	64.76	6
	ATOM	1422	CB	VAL	A	444	12.569	56.869	34.560	1.00	62.76	6

5	ATOM	1423	CG1	VAL	A	444	11.952	58.195	34.174	1.00	64.00	6
	ATOM	1424	CG2	VAL	A	444	12.999	56.891	36.035	1.00	59.27	6
	ATOM	1425	C	VAL	A	444	11.043	55.730	32.861	1.00	68.61	6
	ATOM	1426	O	VAL	A	444	9.937	56.210	32.612	1.00	70.60	8
	ATOM	1427	N	GLU	A	445	11.814	55.173	31.935	1.00	70.71	7
10	ATOM	1428	CA	GLU	A	445	11.457	55.152	30.514	1.00	71.45	6
	ATOM	1429	CB	GLU	A	445	12.725	55.255	29.664	1.00	72.36	6
	ATOM	1430	CG	GLU	A	445	13.598	56.429	30.022	1.00	40.00	6
	ATOM	1431	CD	GLU	A	445	14.875	56.472	29.239	1.00	40.00	6
	ATOM	1432	OE1	GLU	A	445	15.155	55.565	28.414	1.00	40.00	8
15	ATOM	1433	OE2	GLU	A	445	15.663	57.430	29.430	1.00	40.00	8
	ATOM	1434	C	GLU	A	445	10.724	53.912	30.049	1.00	71.46	6
	ATOM	1435	O	GLU	A	445	10.536	53.701	28.844	1.00	73.02	8
	ATOM	1436	N	CYS	A	446	10.301	53.099	30.999	1.00	71.12	7
	ATOM	1437	CA	CYS	A	446	9.628	51.899	30.634	1.00	70.83	6
20	ATOM	1438	CB	CYS	A	446	10.595	50.719	30.687	1.00	71.05	6
	ATOM	1439	SG	CYS	A	446	12.009	50.842	29.573	1.00	72.83	16
	ATOM	1440	C	CYS	A	446	8.454	51.671	31.535	1.00	71.91	6
	ATOM	1441	O	CYS	A	446	8.495	52.014	32.728	1.00	72.06	8
	ATOM	1442	N	PRO	A	447	7.372	51.133	30.978	1.00	73.12	7
25	ATOM	1443	CD	PRO	A	447	7.267	50.764	29.560	1.00	72.88	6
	ATOM	1444	CA	PRO	A	447	6.150	50.853	31.740	1.00	74.22	6
	ATOM	1445	CB	PRO	A	447	5.187	50.281	30.714	1.00	72.98	6
	ATOM	1446	CG	PRO	A	447	5.875	50.271	29.437	1.00	74.77	6
	ATOM	1447	C	PRO	A	447	6.435	49.843	32.831	1.00	75.94	6
30	ATOM	1448	O	PRO	A	447	7.181	48.908	32.612	1.00	76.67	8
	ATOM	1449	N	THR	A	448	5.820	50.002	33.997	1.00	76.91	7
	ATOM	1450	CA	THR	A	448	6.024	49.066	35.113	1.00	78.24	6
	ATOM	1451	CB	THR	A	448	5.528	49.734	36.401	1.00	81.33	6
	ATOM	1452	OG1	THR	A	448	4.105	49.917	36.328	1.00	84.46	8
35	ATOM	1453	CG2	THR	A	448	6.192	51.081	36.585	1.00	83.51	6
	ATOM	1454	C	THR	A	448	5.113	47.912	34.755	1.00	77.42	6
	ATOM	1455	O	THR	A	448	4.915	46.995	35.519	1.00	77.65	8
	ATOM	1456	N	GLU	A	449	4.539	48.021	33.565	1.00	76.29	7
	ATOM	1457	CA	GLU	A	449	3.630	47.023	33.024	1.00	75.03	6
40	ATOM	1458	CB	GLU	A	449	2.600	47.773	32.191	1.00	74.62	6
	ATOM	1459	CG	GLU	A	449	2.145	47.051	31.001	1.00	40.00	6
	ATOM	1460	CD	GLU	A	449	1.297	47.889	30.178	1.00	40.00	6
	ATOM	1461	OE1	GLU	A	449	1.479	49.137	30.146	1.00	40.00	8
	ATOM	1462	OE2	GLU	A	449	0.424	47.322	29.497	1.00	40.00	8
45	ATOM	1463	C	GLU	A	449	4.434	46.036	32.179	1.00	73.49	6
	ATOM	1464	O	GLU	A	449	3.882	45.142	31.559	1.00	70.24	8
	ATOM	1465	N	LEU	A	450	5.747	46.224	32.161	1.00	70.80	7
	ATOM	1466	CA	LEU	A	450	6.608	45.347	31.378	1.00	68.82	6
	ATOM	1467	CB	LEU	A	450	7.301	46.154	30.277	1.00	71.91	6
50	ATOM	1468	CG	LEU	A	450	6.464	46.819	29.217	1.00	76.62	6
	ATOM	1469	CD1	LEU	A	450	7.337	47.662	28.328	1.00	77.95	6
	ATOM	1470	CD2	LEU	A	450	5.786	45.750	28.415	1.00	76.46	6
	ATOM	1471	C	LEU	A	450	7.669	44.673	32.243	1.00	66.22	6
	ATOM	1472	O	LEU	A	450	8.427	43.841	31.752	1.00	66.01	8
55	ATOM	1473	N	PHE	A	451	7.705	45.039	33.530	1.00	61.96	7
	ATOM	1474	CA	PHE	A	451	8.681	44.506	34.480	1.00	58.44	6
	ATOM	1475	CB	PHE	A	451	9.041	45.562	35.540	1.00	61.34	6
	ATOM	1476	CG	PHE	A	451	9.873	46.717	35.008	1.00	63.02	6



5	ATOM	1477	CD1	PHE	A	451	9.426	47.507	33.963	1.00	62.92	6
	ATOM	1478	CD2	PHE	A	451	11.089	47.017	35.593	1.00	63.07	6
	ATOM	1479	CE1	PHE	A	451	10.199	48.598	33.521	1.00	65.12	6
	ATOM	1480	CE2	PHE	A	451	11.860	48.102	35.156	1.00	64.66	6
	ATOM	1481	CZ	PHE	A	451	11.410	48.897	34.118	1.00	67.12	6
10	ATOM	1482	C	PHE	A	451	8.259	43.264	35.260	1.00	56.41	6
	ATOM	1483	O	PHE	A	451	7.641	43.392	36.331	1.00	56.56	8
	ATOM	1484	N	PRO	A	452	8.555	42.045	34.755	1.00	53.28	7
	ATOM	1485	CD	PRO	A	452	9.177	41.689	33.481	1.00	50.46	6
	ATOM	1486	CA	PRO	A	452	8.153	40.859	35.543	1.00	50.26	6
15	ATOM	1487	CB	PRO	A	452	8.739	39.680	34.780	1.00	49.19	6
	ATOM	1488	CG	PRO	A	452	9.178	40.206	33.482	1.00	45.89	6
	ATOM	1489	C	PRO	A	452	8.770	40.999	36.935	1.00	49.62	6
	ATOM	1490	O	PRO	A	452	9.867	41.529	37.094	1.00	52.35	8
	ATOM	1491	N	PRO	A	453	8.139	40.425	37.947	1.00	51.50	7
20	ATOM	1492	CD	PRO	A	453	7.001	39.542	37.797	1.00	49.66	6
	ATOM	1493	CA	PRO	A	453	8.610	40.528	39.323	1.00	50.89	6
	ATOM	1494	CB	PRO	A	453	7.675	39.659	40.109	1.00	51.49	6
	ATOM	1495	CG	PRO	A	453	6.703	39.141	39.185	1.00	50.82	6
	ATOM	1496	C	PRO	A	453	10.015	40.084	39.532	1.00	50.99	6
25	ATOM	1497	O	PRO	A	453	10.876	40.900	39.838	1.00	54.17	8
	ATOM	1498	N	LEU	A	454	10.255	38.781	39.423	1.00	51.21	7
	ATOM	1499	CA	LEU	A	454	11.585	38.298	39.674	1.00	47.17	6
	ATOM	1500	CB	LEU	A	454	11.813	36.962	38.975	1.00	44.44	6
	ATOM	1501	CG	LEU	A	454	13.167	36.375	39.289	1.00	41.33	6
30	ATOM	1502	CD1	LEU	A	454	13.524	36.638	40.720	1.00	35.93	6
	ATOM	1503	CD2	LEU	A	454	13.169	34.907	38.992	1.00	34.79	6
	ATOM	1504	C	LEU	A	454	12.541	39.375	39.182	1.00	42.25	6
	ATOM	1505	O	LEU	A	454	13.477	39.718	39.886	1.00	40.82	8
	ATOM	1506	N	PHE	A	455	12.270	39.957	38.011	1.00	39.29	7
35	ATOM	1507	CA	PHE	A	455	13.133	41.005	37.473	1.00	41.81	6
	ATOM	1508	CB	PHE	A	455	12.527	41.592	36.192	1.00	47.22	6
	ATOM	1509	CG	PHE	A	455	13.433	42.565	35.467	1.00	56.97	6
	ATOM	1510	CD1	PHE	A	455	14.715	42.189	35.135	1.00	57.23	6
	ATOM	1511	CD2	PHE	A	455	12.999	43.840	35.126	1.00	59.40	6
40	ATOM	1512	CE1	PHE	A	455	15.557	43.059	34.466	1.00	56.58	6
	ATOM	1513	CE2	PHE	A	455	13.848	44.716	34.452	1.00	61.80	6
	ATOM	1514	CZ	PHE	A	455	15.129	44.322	34.126	1.00	59.94	6
	ATOM	1515	C	PHE	A	455	13.273	42.085	38.534	1.00	45.12	6
	ATOM	1516	O	PHE	A	455	14.361	42.323	39.034	1.00	39.95	8
45	ATOM	1517	N	LEU	A	456	12.155	42.735	38.849	1.00	43.92	7
	ATOM	1518	CA	LEU	A	456	12.122	43.803	39.840	1.00	44.08	6
	ATOM	1519	CB	LEU	A	456	10.680	44.251	40.093	1.00	50.20	6
	ATOM	1520	CG	LEU	A	456	10.062	45.242	39.144	1.00	55.79	6
	ATOM	1521	CD1	LEU	A	456	8.598	45.432	39.450	1.00	54.70	6
50	ATOM	1522	CD2	LEU	A	456	10.807	46.548	39.295	1.00	53.01	6
	ATOM	1523	C	LEU	A	456	12.739	43.355	41.136	1.00	44.65	6
	ATOM	1524	O	LEU	A	456	13.597	44.022	41.685	1.00	45.93	8
	ATOM	1525	N	GLU	A	457	11.973	41.761	41.851	1.00	44.56	7
	ATOM	1526	CA	GLU	A	457	12.475	41.179	43.105	1.00	46.37	6
55	ATOM	1527	C	GLU	A	457	14.005	41.236	43.132	1.00	43.60	6
	ATOM	1528	O	GLU	A	457	14.583	41.724	44.117	1.00	42.69	8
	ATOM	1529	CB	GLU	A	457	12.024	39.723	43.223	1.00	50.16	6
	ATOM	1530	CG	GLU	A	457	11.114	39.476	44.427	1.00	20.00	6

5	ATOM	1531	CD	GLU	A	457	10.807	37.994	44.648	1.00	20.00	6
	ATOM	1532	OE1	GLU	A	457	11.673	37.099	44.311	1.00	20.00	8
	ATOM	1533	OE2	GLU	A	457	9.683	37.639	45.172	1.00	20.00	8
	ATOM	1534	N	VAL	A	458	14.928	41.078	41.903	1.00	43.21	7
	ATOM	1535	CA	VAL	A	458	16.412	41.094	41.868	1.00	44.98	6
10	ATOM	1536	CB	VAL	A	458	16.881	40.306	40.642	1.00	44.83	6
	ATOM	1537	CG1	VAL	A	458	18.365	40.106	40.698	1.00	49.72	6
	ATOM	1538	CG2	VAL	A	458	16.185	38.979	40.558	1.00	40.89	6
	ATOM	1539	C	VAL	A	458	17.130	42.420	41.877	1.00	42.72	6
	ATOM	1540	O	VAL	A	458	18.061	42.617	42.658	1.00	42.88	8
15	ATOM	1541	N	PHE	A	459	16.713	43.325	41.010	1.00	44.53	7
	ATOM	1542	CA	PHE	A	459	17.385	44.606	40.892	1.00	48.18	6
	ATOM	1543	CB	PHE	A	459	17.281	45.104	39.494	1.00	43.60	6
	ATOM	1544	CG	PHE	A	459	17.915	44.190	38.547	1.00	40.79	6
	ATOM	1545	CD1	PHE	A	459	17.325	42.983	38.244	1.00	41.01	6
20	ATOM	1546	CD2	PHE	A	459	19.153	44.483	38.054	1.00	39.48	6
	ATOM	1547	CE1	PHE	A	459	17.988	42.081	37.441	1.00	40.62	6
	ATOM	1548	CE2	PHE	A	459	19.814	43.589	37.257	1.00	36.87	6
	ATOM	1549	CZ	PHE	A	459	19.233	42.385	36.940	1.00	36.39	6
	ATOM	1550	C	PHE	A	459	16.837	45.648	41.744	1.00	52.71	6
25	ATOM	1551	O	PHE	A	459	17.492	46.682	42.017	1.00	51.34	8
	ATOM	1552	N	GLU	A	460	15.606	45.422	42.161	1.00	62.92	7
	ATOM	1553	CA	GLU	A	460	15.066	46.428	42.965	1.00	69.33	6
	ATOM	1554	CB	GLU	A	460	13.552	46.352	43.094	1.00	72.95	6
	ATOM	1555	CG	GLU	A	460	12.978	47.767	42.957	1.00	78.35	6
30	ATOM	1556	CD	GLU	A	460	12.246	48.261	44.157	1.00	82.97	6
	ATOM	1557	OE1	GLU	A	460	12.471	47.759	45.281	1.00	88.28	8
	ATOM	1558	OE2	GLU	A	460	11.422	49.200	44.017	1.00	84.80	8
	ATOM	1559	C	GLU	A	460	15.736	46.245	44.272	1.00	71.87	6
	ATOM	1560	O	GLU	A	460	16.187	45.170	44.691	1.00	74.51	8
35	ATOM	1561	N	ASP	A	461	15.790	47.373	44.917	1.00	78.50	7
	ATOM	1562	CA	ASP	A	461	16.415	47.505	46.173	1.00	84.19	6
	ATOM	1563	CB	ASP	A	461	16.394	48.981	46.471	1.00	85.82	6
	ATOM	1564	CG	ASP	A	461	16.801	49.786	45.276	1.00	89.62	6
	ATOM	1565	OD1	ASP	A	461	16.692	49.344	44.086	1.00	93.00	8
40	ATOM	1566	OD2	ASP	A	461	17.239	50.923	45.482	1.00	93.04	8
	ATOM	1567	C	ASP	A	461	15.639	46.703	47.214	1.00	86.80	6
	ATOM	1568	O	ASP	A	461	16.245	45.748	47.731	1.00	88.70	8
	ATOM	1569	OXT	ASP	A	461	14.457	47.026	47.451	1.00	88.70	8
	TER											
45	ATOM	1	CB	LYS	B	211	-20.802	66.251	39.780	1.00	46.72	6
	ATOM	2	CG	LYS	B	211	-19.566	65.345	39.922	1.00	56.48	6
	ATOM	3	CD	LYS	B	211	-18.264	66.114	40.045	1.00	60.93	6
	ATOM	4	CE	LYS	B	211	-18.043	67.067	38.886	1.00	61.95	6
	ATOM	5	NZ	LYS	B	211	-19.008	68.224	38.903	1.00	69.93	7
50	ATOM	6	C	LYS	B	211	-22.418	67.861	40.818	1.00	35.68	6
	ATOM	7	O	LYS	B	211	-23.356	67.113	40.454	1.00	33.58	8
	ATOM	8	N	LYS	B	211	-20.742	66.675	42.239	1.00	45.76	7
	ATOM	9	CA	LYS	B	211	-20.998	67.285	40.894	1.00	43.42	6
	ATOM	10	N	PRO	B	212	-22.610	69.205	41.068	1.00	35.64	7
55	ATOM	11	CD	PRO	B	212	-21.526	70.177	41.287	1.00	38.60	6
	ATOM	12	CA	PRO	B	212	-23.943	69.861	41.036	1.00	38.35	6
	ATOM	13	CB	PRO	B	212	-23.657	71.320	41.420	1.00	38.95	6
	ATOM	14	CG	PRO	B	212	-22.226	71.474	41.551	1.00	42.00	6
	ATOM											

5	ATOM	15	C	PRO B 212	-24.798	69.772	39.807	1.00	38.78	6
	ATOM	16	O	PRO B 212	-24.350	70.045	38.696	1.00	34.64	8
	ATOM	17	N	GLU B 213	-26.058	69.424	40.032	1.00	40.31	7
	ATOM	18	CA	GLU B 213	-27.081	69.290	39.003	1.00	43.87	6
	ATOM	19	CB	GLU B 213	-27.895	68.004	39.265	1.00	45.16	6
10	ATOM	20	CG	GLU B 213	-27.032	66.709	39.286	1.00	47.60	6
	ATOM	21	CD	GLU B 213	-27.807	65.421	39.199	1.00	50.68	6
	ATOM	22	OE1	GLU B 213	-28.847	65.244	39.886	1.00	59.18	8
	ATOM	23	OE2	GLU B 213	-27.382	64.516	38.442	1.00	49.06	8
	ATOM	24	C	GLU B 213	-27.924	70.576	39.080	1.00	45.96	6
15	ATOM	25	O	GLU B 213	-27.624	71.467	39.859	1.00	43.13	8
	ATOM	26	N	PRO B 214	-28.987	70.698	38.308	1.00	46.52	7
	ATOM	27	CD	PRO B 214	-29.484	69.635	37.446	1.00	46.44	6
	ATOM	28	CA	PRO B 214	-29.843	71.907	38.302	1.00	47.52	6
	ATOM	29	CB	PRO B 214	-30.799	71.639	37.210	1.00	45.40	6
20	ATOM	30	CG	PRO B 214	-30.530	70.257	36.805	1.00	49.89	6
	ATOM	31	C	PRO B 214	-30.574	72.330	39.535	1.00	45.70	6
	ATOM	32	O	PRO B 214	-30.597	71.595	40.483	1.00	44.49	8
	ATOM	33	N	THR B 215	-31.180	73.515	39.506	1.00	45.24	7
	ATOM	34	CA	THR B 215	-31.965	74.036	40.652	1.00	49.36	6
25	ATOM	35	CB	THR B 215	-31.443	75.420	41.091	1.00	44.86	6
	ATOM	36	OG1	THR B 215	-32.249	76.464	40.534	1.00	52.26	8
	ATOM	37	CG2	THR B 215	-30.011	75.617	40.659	1.00	39.43	6
	ATOM	38	C	THR B 215	-33.386	74.239	40.114	1.00	52.51	6
	ATOM	39	O	THR B 215	-33.562	74.868	39.078	1.00	53.48	8
30	ATOM	40	N	ASP B 216	-34.387	73.741	40.829	1.00	58.81	7
	ATOM	41	CA	ASP B 216	-35.795	73.865	40.435	1.00	61.51	6
	ATOM	42	CB	ASP B 216	-36.674	74.005	41.650	1.00	70.57	6
	ATOM	43	CG	ASP B 216	-37.675	72.981	41.710	1.00	78.07	6
	ATOM	44	OD1	ASP B 216	-38.228	72.588	40.652	1.00	82.31	8
35	ATOM	45	OD2	ASP B 216	-37.983	72.567	42.830	1.00	86.55	8
	ATOM	46	C	ASP B 216	-35.920	75.123	39.648	1.00	58.42	6
	ATOM	47	O	ASP B 216	-36.847	75.317	38.827	1.00	56.85	8
	ATOM	48	N	GLU B 217	-34.954	75.979	39.984	1.00	54.92	7
	ATOM	49	CA	GLU B 217	-34.851	77.259	39.353	1.00	53.37	6
40	ATOM	50	CB	GLU B 217	-34.104	78.264	40.251	1.00	51.02	6
	ATOM	51	CG	GLU B 217	-34.151	79.689	39.679	1.00	40.00	6
	ATOM	52	CD	GLU B 217	-34.301	80.745	40.739	1.00	40.00	6
	ATOM	53	OE1	GLU B 217	-34.089	80.443	41.945	1.00	40.00	8
	ATOM	54	OE2	GLU B 217	-34.625	81.921	40.411	1.00	40.00	8
45	ATOM	55	C	GLU B 217	-34.232	77.163	37.957	1.00	53.55	6
	ATOM	56	O	GLU B 217	-34.815	77.612	37.018	1.00	54.33	8
	ATOM	57	N	GLU B 218	-33.063	76.572	37.839	1.00	49.20	7
	ATOM	58	CA	GLU B 218	-32.318	76.385	36.608	1.00	45.94	6
	ATOM	59	CB	GLU B 218	-30.965	75.793	36.981	1.00	43.43	6
50	ATOM	60	CG	GLU B 218	-30.065	76.728	37.801	1.00	40.86	6
	ATOM	61	CD	GLU B 218	-28.713	76.159	38.072	1.00	39.88	6
	ATOM	62	OE1	GLU B 218	-28.606	74.967	38.449	1.00	37.61	8
	ATOM	63	OE2	GLU B 218	-27.707	76.901	37.945	1.00	34.01	8
	ATOM	64	C	GLU B 218	-33.014	75.475	35.610	1.00	44.71	6
55	ATOM	65	O	GLU B 218	-32.935	75.686	34.405	1.00	45.31	8
	ATOM	66	N	TRP B 219	-33.669	74.439	36.131	1.00	44.02	7
	ATOM	67	CA	TRP B 219	-34.368	73.490	35.290	1.00	46.97	6
	ATOM	68	CB	TRP B 219	-35.046	72.408	36.119	1.00	48.42	6

5	ATOM	69	CG	TRP	B	219	-34.195	71.230	36.374	1.00	54.61	6
	ATOM	70	CD2	TRP	B	219	-34.048	70.120	35.478	1.00	55.24	6
	ATOM	71	CE2	TRP	B	219	-33.076	69.248	36.063	1.00	53.67	6
	ATOM	72	CE3	TRP	B	219	-34.615	69.771	34.252	1.00	54.55	6
	ATOM	73	CD1	TRP	B	219	-33.399	71.019	37.415	1.00	55.75	6
10	ATOM	74	NE1	TRP	B	219	-32.697	69.838	37.236	1.00	54.43	7
	ATOM	75	CZ2	TRP	B	219	-32.635	68.075	35.431	1.00	52.54	6
	ATOM	76	CZ3	TRP	B	219	-34.214	68.603	33.643	1.00	55.17	6
	ATOM	77	CH2	TRP	B	219	-33.234	67.758	34.214	1.00	55.59	6
	ATOM	78	C	TRP	B	219	-35.409	74.199	34.459	1.00	47.32	6
15	ATOM	79	O	TRP	B	219	-35.561	73.914	33.277	1.00	43.56	8
	ATOM	80	N	GLU	B	220	-36.126	75.130	35.084	1.00	49.91	7
	ATOM	81	CA	GLU	B	220	-37.158	75.874	34.402	1.00	53.57	6
	ATOM	82	CB	GLU	B	220	-37.811	76.820	35.373	1.00	58.18	6
	ATOM	83	CG	GLU	B	220	-39.251	76.812	35.221	1.00	73.13	6
20	ATOM	84	CD	GLU	B	220	-39.824	76.858	36.489	1.00	80.06	6
	ATOM	85	OE1	GLU	B	220	-39.485	75.995	37.324	1.00	82.12	8
	ATOM	86	OE2	GLU	B	220	-40.635	77.740	36.718	1.00	82.78	8
	ATOM	87	C	GLU	B	220	-36.539	76.645	33.250	1.00	50.51	6
	ATOM	88	O	GLU	B	220	-37.160	76.793	32.195	1.00	49.94	8
25	ATOM	89	N	LEU	B	221	-35.312	77.135	33.455	1.00	43.71	7
	ATOM	90	CA	LEU	B	221	-34.604	77.884	32.411	1.00	42.81	6
	ATOM	91	CB	LEU	B	221	-33.214	78.324	32.865	1.00	39.21	6
	ATOM	92	CG	LEU	B	221	-32.321	78.833	31.754	1.00	36.34	6
	ATOM	93	CD1	LEU	B	221	-33.073	79.843	30.927	1.00	36.93	6
30	ATOM	94	CD2	LEU	B	221	-31.058	79.446	32.331	1.00	24.18	6
	ATOM	95	C	LEU	B	221	-34.454	77.011	31.192	1.00	43.46	6
	ATOM	96	O	LEU	B	221	-34.819	77.406	30.104	1.00	45.25	8
	ATOM	97	N	ILE	B	222	-33.878	75.829	31.398	1.00	39.09	7
	ATOM	98	CA	ILE	B	222	-33.687	74.857	30.330	1.00	35.47	6
35	ATOM	99	CB	ILE	B	222	-33.224	73.516	30.871	1.00	33.74	6
	ATOM	100	CG2	ILE	B	222	-33.204	72.488	29.776	1.00	28.86	6
	ATOM	101	CG1	ILE	B	222	-31.840	73.631	31.493	1.00	33.33	6
	ATOM	102	CD1	ILE	B	222	-31.435	72.419	32.264	1.00	34.85	6
	ATOM	103	C	ILE	B	222	-34.991	74.627	29.598	1.00	34.26	6
40	ATOM	104	O	ILE	B	222	-35.082	74.832	28.392	1.00	31.90	8
	ATOM	105	N	LYS	B	223	-35.992	74.183	30.346	1.00	39.49	7
	ATOM	106	CA	LYS	B	223	-37.300	73.892	29.785	1.00	44.43	6
	ATOM	107	CB	LYS	B	223	-38.351	73.876	30.882	1.00	50.81	6
	ATOM	108	CG	LYS	B	223	-39.693	73.358	30.411	1.00	62.51	6
45	ATOM	109	CD	LYS	B	223	-40.795	73.532	31.449	1.00	72.22	6
	ATOM	110	CE	LYS	B	223	-42.163	73.249	30.827	1.00	74.55	6
	ATOM	111	NZ	LYS	B	223	-43.268	73.378	31.837	1.00	75.78	7
	ATOM	112	C	LYS	B	223	-37.648	74.942	28.755	1.00	42.81	6
	ATOM	113	O	LYS	B	223	-38.337	74.661	27.796	1.00	40.36	8
50	ATOM	114	N	THR	B	224	-37.146	76.156	28.979	1.00	39.89	7
	ATOM	115	CA	THR	B	224	-37.353	77.293	28.074	1.00	39.93	6
	ATOM	116	CB	THR	B	224	-36.956	78.609	28.776	1.00	40.57	6
	ATOM	117	OG1	THR	B	224	-37.646	78.740	30.028	1.00	39.27	8
	ATOM	118	CG2	THR	B	224	-37.273	79.805	27.893	1.00	38.11	6
55	ATOM	119	C	THR	B	224	-36.521	77.094	26.789	1.00	39.96	6
	ATOM	120	O	THR	B	224	-37.043	76.677	25.756	1.00	36.67	8
	ATOM	121	N	VAL	B	225	-35.231	77.421	26.888	1.00	38.02	7
	ATOM	122	CA	VAL	B	225	-34.263	77.295	25.801	1.00	38.12	6

5	ATOM	123	CB	VAL	B	225	-32.869	77.015	26.348	1.00	38.19	6
	ATOM	124	CG1	VAL	B	225	-31.863	76.983	25.226	1.00	36.77	6
	ATOM	125	CG2	VAL	B	225	-32.483	78.050	27.353	1.00	41.76	6
	ATOM	126	C	VAL	B	225	-34.656	76.191	24.843	1.00	37.52	6
	ATOM	127	O	VAL	B	225	-34.621	76.364	23.638	1.00	36.77	8
10	ATOM	128	N	THR	B	226	-35.005	75.046	25.410	1.00	34.02	7
	ATOM	129	CA	THR	B	226	-35.423	73.887	24.638	1.00	34.67	6
	ATOM	130	CB	THR	B	226	-35.677	72.707	25.574	1.00	30.56	6
	ATOM	131	OG1	THR	B	226	-34.432	72.225	26.084	1.00	32.20	8
	ATOM	132	CG2	THR	B	226	-36.413	71.595	24.874	1.00	20.99	6
15	ATOM	133	C	THR	B	226	-36.664	74.170	23.803	1.00	36.41	6
	ATOM	134	O	THR	B	226	-36.633	74.054	22.578	1.00	39.64	8
	ATOM	135	N	ALA	B	227	-37.746	74.542	24.480	1.00	39.20	7
	ATOM	136	CA	ALA	B	227	-39.008	74.861	23.822	1.00	36.93	6
	ATOM	137	CB	ALA	B	227	-39.914	75.631	24.785	1.00	38.06	6
20	ATOM	138	C	ALA	B	227	-38.686	75.719	22.608	1.00	37.69	6
	ATOM	139	O	ALA	B	227	-39.317	75.616	21.566	1.00	40.94	8
	ATOM	140	N	ALA	B	228	-37.677	76.572	22.785	1.00	32.86	7
	ATOM	141	CA	ALA	B	228	-37.216	77.483	21.753	1.00	32.48	6
	ATOM	142	CB	ALA	B	228	-36.252	78.458	22.358	1.00	28.25	6
25	ATOM	143	C	ALA	B	228	-36.545	76.704	20.638	1.00	36.12	6
	ATOM	144	O	ALA	B	228	-37.078	76.586	19.544	1.00	37.86	8
	ATOM	145	N	HIS	B	229	-35.364	76.175	20.924	1.00	33.58	7
	ATOM	146	CA	HIS	B	229	-34.611	75.409	19.956	1.00	32.97	6
	ATOM	147	CB	HIS	B	229	-33.418	74.721	20.597	1.00	33.69	6
30	ATOM	148	CG	HIS	B	229	-32.776	73.714	19.715	1.00	28.39	6
	ATOM	149	CD2	HIS	B	229	-32.535	72.384	19.863	1.00	28.83	6
	ATOM	150	ND1	HIS	B	229	-32.336	74.030	18.426	1.00	30.47	7
	ATOM	151	CE1	HIS	B	229	-31.867	72.929	17.855	1.00	26.95	6
	ATOM	152	NE2	HIS	B	229	-31.976	71.927	18.700	1.00	31.27	7
35	ATOM	153	C	HIS	B	229	-35.362	74.352	19.202	1.00	38.40	6
	ATOM	154	O	HIS	B	229	-35.069	74.131	18.045	1.00	41.49	8
	ATOM	155	N	VAL	B	230	-36.296	73.688	19.882	1.00	38.55	7
	ATOM	156	CA	VAL	B	230	-37.077	72.634	19.263	1.00	40.40	6
	ATOM	157	CB	VAL	B	230	-37.744	71.747	20.310	1.00	44.68	6
40	ATOM	158	CG1	VAL	B	230	-38.381	70.537	19.637	1.00	39.39	6
	ATOM	159	CG2	VAL	B	230	-36.742	71.311	21.356	1.00	42.18	6
	ATOM	160	C	VAL	B	230	-38.133	73.130	18.284	1.00	44.28	6
	ATOM	161	O	VAL	B	230	-38.375	72.505	17.248	1.00	45.94	8
	ATOM	162	N	ALA	B	231	-38.774	74.240	18.623	1.00	45.59	7
45	ATOM	163	CA	ALA	B	231	-39.820	74.804	17.792	1.00	47.84	6
	ATOM	164	CB	ALA	B	231	-40.736	75.661	18.647	1.00	45.08	6
	ATOM	165	C	ALA	B	231	-39.235	75.636	16.673	1.00	48.04	6
	ATOM	166	O	ALA	B	231	-39.959	76.128	15.816	1.00	49.95	8
	ATOM	167	N	THR	B	232	-37.914	75.773	16.669	1.00	47.26	7
50	ATOM	168	CA	THR	B	232	-37.220	76.563	15.654	1.00	43.64	6
	ATOM	169	CB	THR	B	232	-36.482	77.746	16.315	1.00	41.93	6
	ATOM	170	OG1	THR	B	232	-35.385	77.270	17.098	1.00	39.10	8
	ATOM	171	CG2	THR	B	232	-37.423	78.523	17.232	1.00	29.80	6
	ATOM	172	C	THR	B	232	-36.194	75.719	14.914	1.00	43.97	6
55	ATOM	173	O	THR	B	232	-35.401	76.252	14.155	1.00	40.55	8
	ATOM	174	N	ASN	B	233	-36.195	74.407	15.157	1.00	48.62	7
	ATOM	175	CA	ASN	B	233	-35.247	73.511	14.483	1.00	58.62	6
	ATOM	176	CB	ASN	B	233	-34.621	72.537	15.500	1.00	62.44	6

5	ATOM	177	CG	ASN	B	233	-33.407	71.812	14.946	1.00	68.35	6
	ATOM	178	OD1	ASN	B	233	-32.569	72.427	14.256	1.00	65.50	8
	ATOM	179	ND2	ASN	B	233	-33.288	70.529	15.265	1.00	74.29	7
	ATOM	180	C	ASN	B	233	-36.033	72.755	13.437	1.00	65.06	6
	ATOM	181	O	ASN	B	233	-36.950	72.005	13.754	1.00	69.47	8
10	ATOM	182	N	ALA	B	234	-35.674	72.986	12.182	1.00	68.80	7
	ATOM	183	CA	ALA	B	234	-36.352	72.376	11.036	1.00	70.98	6
	ATOM	184	CB	ALA	B	234	-35.585	72.701	9.769	1.00	71.43	6
	ATOM	185	C	ALA	B	234	-36.556	70.880	11.111	1.00	73.83	6
	ATOM	186	O	ALA	B	234	-35.677	70.142	11.501	1.00	74.33	8
15	ATOM	187	N	GLN	B	235	-37.754	70.479	10.717	1.00	75.07	7
	ATOM	188	CA	GLN	B	235	-38.149	69.095	10.690	1.00	76.32	6
	ATOM	189	CB	GLN	B	235	-37.468	68.365	9.533	1.00	76.98	6
	ATOM	190	CG	GLN	B	235	-38.120	68.540	8.170	1.00	77.07	6
	ATOM	191	CD	GLN	B	235	-38.572	69.940	7.909	1.00	80.85	6
20	ATOM	192	OE1	GLN	B	235	-39.575	70.401	8.491	1.00	82.01	8
	ATOM	193	NE2	GLN	B	235	-37.862	70.620	7.040	1.00	78.80	7
	ATOM	194	C	GLN	B	235	-37.904	68.331	11.953	1.00	77.15	6
	ATOM	195	O	GLN	B	235	-38.087	67.137	11.947	1.00	76.06	8
	ATOM	196	N	GLY	B	236	-37.511	68.985	13.039	1.00	77.46	7
25	ATOM	197	CA	GLY	B	236	-37.304	68.263	14.288	1.00	78.37	6
	ATOM	198	C	GLY	B	236	-36.717	66.882	14.217	1.00	79.43	6
	ATOM	199	O	GLY	B	236	-35.717	66.650	13.542	1.00	79.47	8
	ATOM	200	N	SER	B	237	-37.420	66.007	14.943	1.00	77.98	7
	ATOM	201	CA	SER	B	237	-37.117	64.600	15.092	1.00	76.49	6
30	ATOM	202	CB	SER	B	237	-38.118	63.953	16.066	1.00	76.46	6
	ATOM	203	C	SER	B	237	-37.181	63.895	13.737	1.00	75.35	6
	ATOM	204	O	SER	B	237	-36.493	62.911	13.524	1.00	75.47	8
	ATOM	205	N	HIS	B	238	-38.004	64.443	12.845	1.00	75.56	7
	ATOM	206	CA	HIS	B	238	-38.293	63.926	11.519	1.00	75.46	6
35	ATOM	207	CB	HIS	B	238	-39.663	64.397	11.096	1.00	75.85	6
	ATOM	208	C	HIS	B	238	-37.369	64.216	10.380	1.00	74.10	6
	ATOM	209	O	HIS	B	238	-37.747	64.135	9.222	1.00	75.34	8
	ATOM	210	N	TRP	B	239	-36.127	64.427	10.651	1.00	73.39	7
	ATOM	211	CA	TRP	B	239	-35.345	64.786	9.519	1.00	74.02	6
40	ATOM	212	CB	TRP	B	239	-34.121	65.542	9.934	1.00	81.77	6
	ATOM	213	CG	TRP	B	239	-33.085	64.786	10.737	1.00	89.67	6
	ATOM	214	CD2	TRP	B	239	-31.727	64.530	10.302	1.00	93.19	6
	ATOM	215	CE2	TRP	B	239	-31.069	63.848	11.393	1.00	95.46	6
	ATOM	216	CE3	TRP	B	239	-30.949	64.941	9.196	1.00	95.35	6
45	ATOM	217	CD1	TRP	B	239	-33.237	64.180	11.926	1.00	94.16	6
	ATOM	218	NE1	TRP	B	239	-32.022	63.631	12.347	1.00	97.48	7
	ATOM	219	CZ2	TRP	B	239	-29.706	63.475	11.348	1.00	96.23	6
	ATOM	220	CZ3	TRP	B	239	-29.613	64.533	9.128	1.00	96.75	6
	ATOM	221	CH2	TRP	B	239	-28.978	63.870	10.215	1.00	97.32	6
50	ATOM	222	C	TRP	B	239	-34.994	63.722	8.539	1.00	70.77	6
	ATOM	223	O	TRP	B	239	-35.423	63.772	7.388	1.00	71.70	8
	ATOM	224	N	LYS	B	240	-34.165	62.791	8.955	1.00	67.10	7
	ATOM	225	CA	LYS	B	240	-33.724	61.744	8.077	1.00	65.63	6
	ATOM	226	CB	LYS	B	240	-33.321	60.539	8.906	1.00	66.65	6
55	ATOM	227	CG	LYS	B	240	-32.210	60.824	9.905	1.00	69.83	6
	ATOM	228	CD	LYS	B	240	-31.759	59.553	10.602	1.00	71.49	6
	ATOM	229	CE	LYS	B	240	-30.576	59.843	11.493	1.00	71.31	6
	ATOM	230	NZ	LYS	B	240	-30.106	58.604	12.157	1.00	72.23	7

5	ATOM	231	C	LYS B 240	-34.719	61.331	6.996	1.00	66.19	6
	ATOM	232	O	LYS B 240	-34.321	60.673	6.031	1.00	65.20	8
	ATOM	233	N	ASN B 241	-35.986	61.727	7.139	1.00	66.69	7
	ATOM	234	CA	ASN B 241	-37.031	61.393	6.171	1.00	67.53	6
	ATOM	235	CB	ASN B 241	-38.240	60.846	6.915	1.00	67.98	6
10	ATOM	236	CG	ASN B 241	-37.966	59.479	7.544	1.00	70.19	6
	ATOM	237	OD1	ASN B 241	-37.561	58.526	6.845	1.00	71.37	8
	ATOM	238	ND2	ASN B 241	-38.205	59.370	8.836	1.00	71.48	7
	ATOM	239	C	ASN B 241	-37.496	62.532	5.255	1.00	66.62	6
	ATOM	240	O	ASN B 241	-38.504	62.395	4.578	1.00	64.76	8
15	ATOM	241	N	LYS B 242	-36.753	63.633	5.209	1.00	66.86	7
	ATOM	242	CA	LYS B 242	-37.096	64.772	4.362	1.00	67.46	6
	ATOM	243	CB	LYS B 242	-37.501	65.948	5.258	1.00	67.93	6
	ATOM	244	CG	LYS B 242	-38.746	65.684	6.076	1.00	71.52	6
	ATOM	245	CD	LYS B 242	-40.007	65.528	5.215	1.00	74.32	6
20	ATOM	246	CE	LYS B 242	-40.416	66.852	4.564	1.00	74.41	6
	ATOM	247	NZ	LYS B 242	-40.657	67.941	5.575	1.00	74.44	7
	ATOM	248	C	LYS B 242	-35.826	65.081	3.592	1.00	66.28	6
	ATOM	249	O	LYS B 242	-35.814	65.799	2.601	1.00	67.61	8
	ATOM	250	N	ARG B 243	-34.763	64.485	4.112	1.00	64.19	7
25	ATOM	251	CA	ARG B 243	-33.410	64.577	3.591	1.00	62.43	6
	ATOM	252	CB	ARG B 243	-32.599	63.547	4.390	1.00	60.12	6
	ATOM	253	CG	ARG B 243	-31.128	63.558	4.171	1.00	40.00	6
	ATOM	254	CD	ARG B 243	-30.335	62.888	5.319	1.00	40.00	6
	ATOM	255	NE	ARG B 243	-30.269	61.428	5.296	1.00	40.00	7
30	ATOM	256	CZ	ARG B 243	-29.384	60.724	6.009	1.00	40.00	6
	ATOM	257	NH1	ARG B 243	-28.510	61.357	6.798	1.00	40.00	7
	ATOM	258	NH2	ARG B 243	-29.355	59.401	5.908	1.00	40.00	7
	ATOM	259	C	ARG B 243	-33.408	64.252	2.100	1.00	62.97	6
	ATOM	260	O	ARG B 243	-33.690	63.122	1.722	1.00	63.96	8
35	ATOM	261	N	LYS B 244	-33.105	65.245	1.270	1.00	62.41	7
	ATOM	262	CA	LYS B 244	-33.054	65.053	-0.179	1.00	61.57	6
	ATOM	263	CB	LYS B 244	-34.104	65.941	-0.866	1.00	63.68	6
	ATOM	264	CG	LYS B 244	-35.527	65.731	-0.337	1.00	71.29	6
	ATOM	265	CD	LYS B 244	-36.566	66.549	-1.107	1.00	73.83	6
40	ATOM	266	CE	LYS B 244	-36.219	68.045	-1.138	1.00	74.71	6
	ATOM	267	NZ	LYS B 244	-36.169	68.689	0.219	1.00	73.32	7
	ATOM	268	C	LYS B 244	-31.658	65.402	-0.670	1.00	59.30	6
	ATOM	269	O	LYS B 244	-31.317	66.570	-0.852	1.00	56.34	8
	ATOM	270	N	PHE B 245	-30.858	64.359	-0.875	1.00	57.06	7
45	ATOM	271	CA	PHE B 245	-29.462	64.525	-1.305	1.00	59.01	6
	ATOM	272	CB	PHE B 245	-28.786	63.179	-1.478	1.00	59.62	6
	ATOM	273	CG	PHE B 245	-28.991	62.288	-0.339	1.00	66.60	6
	ATOM	274	CD1	PHE B 245	-30.200	61.669	-0.172	1.00	67.17	6
	ATOM	275	CD2	PHE B 245	-28.012	62.117	0.593	1.00	69.25	6
50	ATOM	276	CE1	PHE B 245	-30.404	60.882	0.911	1.00	69.92	6
	ATOM	277	CE2	PHE B 245	-28.229	61.329	1.669	1.00	70.50	6
	ATOM	278	CZ	PHE B 245	-29.418	60.714	1.830	1.00	70.89	6
	ATOM	279	C	PHE B 245	-29.301	65.282	-2.592	1.00	60.68	6
	ATOM	280	O	PHE B 245	-29.859	64.911	-3.619	1.00	62.37	8
55	ATOM	281	N	LEU B 246	-28.495	66.336	-2.505	1.00	60.10	7
	ATOM	282	CA	LEU B 246	-28.201	67.199	-3.631	1.00	59.44	6
	ATOM	283	CB	LEU B 246	-27.248	68.332	-3.231	1.00	57.43	6
	ATOM	284	CG	LEU B 246	-27.118	69.474	-4.207	1.00	54.41	6

5	ATOM	285	CD1	LEU B 246	-28.481	70.137	-4.349	1.00	52.43	6
	ATOM	286	CD2	LEU B 246	-26.112	70.470	-3.719	1.00	51.69	6
	ATOM	287	C	LEU B 246	-27.585	66.379	-4.740	1.00	62.05	6
	ATOM	288	O	LEU B 246	-26.789	65.446	-4.486	1.00	59.85	8
	ATOM	289	N	PRO B 247	-27.930	66.693	-5.984	1.00	63.33	7
10	ATOM	290	CD	PRO B 247	-28.839	67.781	-6.363	1.00	64.44	6
	ATOM	291	CA	PRO B 247	-27.391	65.958	-7.130	1.00	63.56	6
	ATOM	292	CB	PRO B 247	-27.976	66.675	-8.340	1.00	64.42	6
	ATOM	293	CG	PRO B 247	-28.873	67.714	-7.841	1.00	64.90	6
	ATOM	294	C	PRO B 247	-25.866	65.947	-7.143	1.00	61.94	6
15	ATOM	295	O	PRO B 247	-25.223	66.944	-6.856	1.00	61.60	8
	ATOM	296	N	GLU B 248	-25.333	64.771	-7.478	1.00	61.33	7
	ATOM	297	CA	GLU B 248	-23.896	64.516	-7.590	1.00	63.50	6
	ATOM	298	CB	GLU B 248	-23.630	63.154	-8.248	1.00	66.94	6
	ATOM	299	CG	GLU B 248	-22.168	62.953	-8.713	1.00	68.70	6
20	ATOM	300	CD	GLU B 248	-21.898	61.745	-9.580	1.00	40.00	6
	ATOM	301	OE1	GLU B 248	-22.863	61.007	-10.035	1.00	40.00	8
	ATOM	302	OE2	GLU B 248	-20.709	61.460	-9.838	1.00	40.00	8
	ATOM	303	C	GLU B 248	-23.158	65.571	-8.415	1.00	64.19	6
	ATOM	304	O	GLU B 248	-22.056	65.975	-8.066	1.00	65.56	8
25	ATOM	305	N	ASP B 249	-23.796	66.019	-9.498	1.00	64.36	7
	ATOM	306	CA	ASP B 249	-23.254	66.994	-10.436	1.00	63.33	6
	ATOM	307	CB	ASP B 249	-24.122	67.031	-11.698	1.00	62.97	6
	ATOM	308	CG	ASP B 249	-25.437	67.715	-11.489	1.00	64.63	6
	ATOM	309	OD1	ASP B 249	-26.235	67.285	-10.629	1.00	64.84	8
30	ATOM	310	OD2	ASP B 249	-25.726	68.718	-12.189	1.00	66.52	8
	ATOM	311	C	ASP B 249	-23.068	68.413	-9.960	1.00	64.31	6
	ATOM	312	O	ASP B 249	-22.117	69.084	-10.355	1.00	64.73	8
	ATOM	313	N	ILE B 250	-23.987	68.892	-9.136	1.00	63.09	7
	ATOM	314	CA	ILE B 250	-23.921	70.281	-8.660	1.00	64.39	6
35	ATOM	315	CB	ILE B 250	-25.124	70.575	-7.798	1.00	65.79	6
	ATOM	316	CG2	ILE B 250	-25.559	72.041	-7.858	1.00	64.78	6
	ATOM	317	CG1	ILE B 250	-26.348	69.752	-8.206	1.00	65.28	6
	ATOM	318	CD1	ILE B 250	-27.671	70.444	-7.887	1.00	65.08	6
	ATOM	319	C	ILE B 250	-22.815	70.488	-7.714	1.00	65.21	6
40	ATOM	320	O	ILE B 250	-22.754	69.847	-6.656	1.00	64.05	8
	ATOM	321	N	GLY B 251	-22.024	71.392	-8.103	1.00	65.48	7
	ATOM	322	CA	GLY B 251	-20.873	71.721	-7.342	1.00	67.32	6
	ATOM	323	C	GLY B 251	-19.808	70.806	-7.800	1.00	68.52	6
	ATOM	324	O	GLY B 251	-19.791	70.548	-9.025	1.00	65.49	8
45	ATOM	325	N	GLN B 252	-19.074	70.440	-6.799	1.00	72.26	7
	ATOM	326	CA	GLN B 252	-17.949	69.540	-6.883	1.00	74.10	6
	ATOM	327	CB	GLN B 252	-18.460	68.098	-6.723	1.00	75.82	6
	ATOM	328	CG	GLN B 252	-17.367	67.088	-6.356	1.00	77.81	6
	ATOM	329	CD	GLN B 252	-17.924	65.759	-5.824	1.00	79.38	6
50	ATOM	330	OE1	GLN B 252	-18.615	65.042	-6.549	1.00	80.55	8
	ATOM	331	NE2	GLN B 252	-17.661	65.380	-4.586	1.00	78.12	7
	ATOM	332	C	GLN B 252	-17.258	69.727	-8.258	1.00	77.17	6
	ATOM	333	O	GLN B 252	-17.977	70.009	-9.227	1.00	76.50	8
	ATOM	334	N	ALA B 253	-15.718	69.795	-8.279	1.00	80.78	7
55	ATOM	335	CA	ALA B 253	-14.615	70.766	-8.544	1.00	83.70	6
	ATOM	336	CB	ALA B 253	-13.794	70.914	-7.255	1.00	83.23	6
	ATOM	337	C	ALA B 253	-13.605	70.732	-9.731	1.00	85.59	6
	ATOM	338	O	ALA B 253	-13.186	69.691	-10.171	1.00	85.69	8



5	ATOM	339	N	PRO B 254	-13.223	71.944	-10.246	1.00	35.05	7
	ATOM	340	CD	PRO B 254	-13.798	73.217	-9.752	1.00	33.97	6
	ATOM	341	CA	PRO B 254	-12.266	72.177	-11.351	1.00	35.89	6
	ATOM	342	CB	PRO B 254	-12.275	73.710	-11.596	1.00	33.94	6
	ATOM	343	CG	PRO B 254	-13.222	74.277	-10.688	1.00	33.31	6
10	ATOM	344	C	PRO B 254	-10.827	71.665	-11.121	1.00	37.75	6
	ATOM	345	O	PRO B 254	-10.379	71.426	-10.009	1.00	38.78	8
	TER									
	ATOM	1	N	GLY B 261	-8.238	79.356	-2.979	1.00	40.00	7
	ATOM	2	CA	GLY B 261	-9.314	78.411	-3.005	1.00	40.00	6
15	ATOM	3	C	GLY B 261	-10.206	78.717	-4.355	1.00	40.00	6
	ATOM	4	O	GLY B 261	-11.372	79.141	-4.256	1.00	40.00	8
	ATOM	5	N	GLY B 262	-9.565	78.527	-5.597	1.00	40.00	7
	ATOM	6	CA	GLY B 262	-10.136	78.609	-7.087	1.00	40.00	6
	ATOM	7	C	GLY B 262	-10.849	79.966	-7.577	1.00	40.00	6
20	ATOM	8	O	GLY B 262	-10.200	81.044	-7.543	1.00	40.00	8
	ATOM	9	N	LYS B 263	-12.086	79.687	-8.124	1.00	61.71	7
	ATOM	10	CA	LYS B 263	-13.323	80.536	-8.428	1.00	64.36	6
	ATOM	11	C	LYS B 263	-14.367	79.750	-7.614	1.00	63.41	6
	ATOM	12	O	LYS B 263	-14.102	78.579	-7.280	1.00	61.93	8
25	ATOM	13	CB	LYS B 263	-13.901	80.405	-9.876	1.00	63.50	6
	ATOM	14	CG	LYS B 263	-13.487	81.474	-10.881	1.00	20.00	6
	ATOM	15	CD	LYS B 263	-14.016	82.897	-10.612	1.00	20.00	6
	ATOM	16	CE	LYS B 263	-13.641	83.874	-11.742	1.00	20.00	6
	ATOM	17	NZ	LYS B 263	-13.680	85.287	-11.341	1.00	20.00	7
30	ATOM	18	N	VAL B 264	-15.489	80.335	-7.307	1.00	61.15	7
	ATOM	19	CA	VAL B 264	-16.616	79.632	-6.619	1.00	59.46	6
	ATOM	20	CB	VAL B 264	-17.574	80.703	-6.099	1.00	59.03	6
	ATOM	21	CG1	VAL B 264	-18.479	80.215	-4.979	1.00	53.79	6
	ATOM	22	CG2	VAL B 264	-16.847	81.938	-5.562	1.00	55.32	6
35	ATOM	23	C	VAL B 264	-17.330	78.824	-7.700	1.00	60.96	6
	ATOM	24	O	VAL B 264	-16.940	78.873	-8.873	1.00	62.13	8
	ATOM	25	N	ASP B 265	-18.378	78.098	-7.340	1.00	62.59	7
	ATOM	26	CA	ASP B 265	-19.175	77.339	-8.312	1.00	64.95	6
	ATOM	27	CB	ASP B 265	-18.796	75.851	-8.270	1.00	64.32	6
40	ATOM	28	CG	ASP B 265	-19.928	75.022	-8.584	1.00	67.70	6
	ATOM	29	OD1	ASP B 265	-20.856	75.062	-9.295	1.00	72.59	8
	ATOM	30	OD2	ASP B 265	-20.370	73.959	-8.310	1.00	68.84	8
	ATOM	31	C	ASP B 265	-20.658	77.614	-8.016	1.00	65.64	6
	ATOM	32	O	ASP B 265	-21.342	76.895	-7.313	1.00	68.81	8
45	ATOM	33	N	LEU B 266	-21.066	78.737	-8.588	1.00	65.12	7
	ATOM	34	CA	LEU B 266	-22.385	79.330	-8.499	1.00	63.40	6
	ATOM	35	CB	LEU B 266	-22.429	80.448	-9.542	1.00	67.34	6
	ATOM	36	CG	LEU B 266	-21.295	81.459	-9.399	1.00	69.35	6
	ATOM	37	CD1	LEU B 266	-20.983	82.127	-10.712	1.00	68.24	6
50	ATOM	38	CD2	LEU B 266	-21.663	82.461	-8.344	1.00	70.47	6
	ATOM	39	C	LEU B 266	-23.673	78.507	-8.602	1.00	59.67	6
	ATOM	40	O	LEU B 266	-24.684	78.890	-7.988	1.00	53.35	8
	ATOM	41	N	GLU B 267	-23.677	77.416	-9.371	1.00	58.01	7
	ATOM	42	CA	GLU B 267	-24.901	76.640	-9.449	1.00	58.34	6
55	ATOM	43	CB	GLU B 267	-24.752	75.410	-10.368	1.00	59.21	6
	ATOM	44	CG	GLU B 267	-25.979	74.464	-10.268	1.00	62.89	6
	ATOM	45	CD	GLU B 267	-26.048	73.419	-11.328	1.00	67.66	6
	ATOM	46	OE1	GLU B 267	-25.076	72.645	-11.512	1.00	69.95	8

5	ATOM	47	OE2	GLU	B	267	-27.098	73.328	-12.008	1.00	69.40	8
	ATOM	48	C	GLU	B	267	-25.200	76.184	-8.032	1.00	57.67	6
	ATOM	49	O	GLU	B	267	-26.354	76.009	-7.643	1.00	58.34	8
	ATOM	50	N	ALA	B	268	-24.114	75.996	-7.285	1.00	53.43	7
	ATOM	51	CA	ALA	B	268	-24.151	75.560	-5.905	1.00	49.00	6
10	ATOM	52	CB	ALA	B	268	-22.816	74.956	-5.526	1.00	45.72	6
	ATOM	53	C	ALA	B	268	-24.421	76.775	-5.056	1.00	45.76	6
	ATOM	54	O	ALA	B	268	-25.419	76.823	-4.351	1.00	41.50	8
	ATOM	55	N	PHE	B	269	-23.533	77.766	-5.142	1.00	41.43	7
	ATOM	56	CA	PHE	B	269	-23.688	78.989	-4.358	1.00	43.96	6
15	ATOM	57	CB	PHE	B	269	-22.903	80.150	-4.971	1.00	40.10	6
	ATOM	58	CG	PHE	B	269	-23.057	81.458	-4.224	1.00	40.44	6
	ATOM	59	CD1	PHE	B	269	-22.284	81.727	-3.105	1.00	38.98	6
	ATOM	60	CD2	PHE	B	269	-24.033	82.372	-4.603	1.00	37.15	6
	ATOM	61	CE1	PHE	B	269	-22.472	82.921	-2.388	1.00	32.12	6
20	ATOM	62	CE2	PHE	B	269	-24.228	83.567	-3.890	1.00	38.41	6
	ATOM	63	CZ	PHE	B	269	-23.457	83.838	-2.780	1.00	40.55	6
	ATOM	64	C	PHE	B	269	-25.154	79.374	-4.320	1.00	49.76	6
	ATOM	65	O	PHE	B	269	-25.645	79.905	-3.336	1.00	52.15	8
	ATOM	66	N	SER	B	270	-25.840	79.112	-5.426	1.00	53.15	7
25	ATOM	67	CA	SER	B	270	-27.253	79.431	-5.520	1.00	52.29	6
	ATOM	68	CB	SER	B	270	-27.742	79.274	-6.948	1.00	51.85	6
	ATOM	69	OG	SER	B	270	-29.118	79.606	-7.048	1.00	53.42	8
	ATOM	70	C	SER	B	270	-28.012	78.486	-4.630	1.00	49.38	6
	ATOM	71	O	SER	B	270	-28.438	78.864	-3.548	1.00	48.74	8
30	ATOM	72	N	HIS	B	271	-28.185	77.253	-5.115	1.00	50.15	7
	ATOM	73	CA	HIS	B	271	-28.904	76.203	-4.382	1.00	51.67	6
	ATOM	74	CB	HIS	B	271	-28.409	74.812	-4.782	1.00	58.52	6
	ATOM	75	CG	HIS	B	271	-29.096	74.248	-5.976	1.00	68.97	6
	ATOM	76	CD2	HIS	B	271	-29.987	73.233	-6.102	1.00	70.88	6
35	ATOM	77	ND1	HIS	B	271	-28.943	74.770	-7.270	1.00	71.98	7
	ATOM	78	CE1	HIS	B	271	-29.716	74.080	-8.100	1.00	73.91	6
	ATOM	79	NE2	HIS	B	271	-30.354	73.149	-7.419	1.00	73.59	7
	ATOM	80	C	HIS	B	271	-28.785	76.347	-2.886	1.00	48.33	6
	ATOM	81	O	HIS	B	271	-29.641	75.874	-2.156	1.00	48.39	8
40	ATOM	82	N	PHE	B	272	-27.702	76.992	-2.444	1.00	41.34	7
	ATOM	83	CA	PHE	B	272	-27.440	77.224	-1.033	1.00	39.44	6
	ATOM	84	CB	PHE	B	272	-25.936	77.302	-0.801	1.00	36.67	6
	ATOM	85	CG	PHE	B	272	-25.241	75.945	-0.861	1.00	33.39	6
	ATOM	86	CD1	PHE	B	272	-23.856	75.857	-0.976	1.00	33.14	6
45	ATOM	87	CD2	PHE	B	272	-25.973	74.767	-0.732	1.00	38.28	6
	ATOM	88	CE1	PHE	B	272	-23.200	74.606	-0.989	1.00	38.26	6
	ATOM	89	CE2	PHE	B	272	-25.321	73.518	-0.743	1.00	43.28	6
	ATOM	90	CZ	PHE	B	272	-23.937	73.441	-0.856	1.00	39.74	6
	ATOM	91	C	PHE	B	272	-28.144	78.472	-0.477	1.00	40.75	6
50	ATOM	92	O	PHE	B	272	-28.803	78.393	0.558	1.00	35.51	8
	ATOM	93	N	THR	B	273	-28.027	79.621	-1.144	1.00	41.64	7
	ATOM	94	CA	THR	B	273	-28.658	80.850	-0.652	1.00	45.97	6
	ATOM	95	CB	THR	B	273	-28.023	82.105	-1.283	1.00	51.52	6
	ATOM	96	OG1	THR	B	273	-28.292	82.151	-2.688	1.00	45.74	8
55	ATOM	97	CG2	THR	B	273	-26.511	82.123	-1.048	1.00	49.73	6
	ATOM	98	C	THR	B	273	-30.142	80.859	-0.971	1.00	46.23	6
	ATOM	99	O	THR	B	273	-30.862	81.751	-0.535	1.00	41.21	8
	ATOM	100	N	LYS	B	274	-30.583	79.876	-1.758	1.00	46.21	7

5	ATOM	101	CA	LYS	B	274	-31.983	79.774	-2.147	1.00	54.53	6
	ATOM	102	CB	LYS	B	274	-32.133	78.724	-3.232	1.00	54.36	6
	ATOM	103	C	LYS	B	274	-32.819	79.396	-0.931	1.00	56.88	6
	ATOM	104	O	LYS	B	274	-34.025	79.624	-0.906	1.00	57.98	8
	ATOM	105	N	ILE	B	275	-32.151	78.820	0.076	1.00	56.48	7
10	ATOM	106	CA	ILE	B	275	-32.791	78.381	1.332	1.00	52.64	6
	ATOM	107	CB	ILE	B	275	-32.638	76.863	1.519	1.00	49.15	6
	ATOM	108	CG2	ILE	B	275	-33.505	76.105	0.529	1.00	47.42	6
	ATOM	109	CG1	ILE	B	275	-31.188	76.441	1.343	1.00	45.31	6
	ATOM	110	CD1	ILE	B	275	-30.990	74.952	1.391	1.00	37.22	6
15	ATOM	111	C	ILE	B	275	-32.241	79.086	2.574	1.00	51.78	6
	ATOM	112	O	ILE	B	275	-32.858	79.049	3.622	1.00	49.80	8
	ATOM	113	N	ILE	B	276	-31.071	79.709	2.435	1.00	51.76	7
	ATOM	114	CA	ILE	B	276	-30.410	80.409	3.533	1.00	52.58	6
	ATOM	115	CB	ILE	B	276	-29.145	81.110	3.042	1.00	55.04	6
20	ATOM	116	CG2	ILE	B	276	-29.486	82.172	2.017	1.00	53.28	6
	ATOM	117	CG1	ILE	B	276	-28.396	81.786	4.203	1.00	57.31	6
	ATOM	118	CD1	ILE	B	276	-27.862	80.854	5.231	1.00	60.32	6
	ATOM	119	C	ILE	B	276	-31.282	81.461	4.237	1.00	50.70	6
	ATOM	120	O	ILE	B	276	-31.015	81.817	5.385	1.00	55.55	8
25	ATOM	121	N	THR	B	277	-32.322	81.953	3.568	1.00	47.33	7
	ATOM	122	CA	THR	B	277	-33.174	82.968	4.141	1.00	42.59	6
	ATOM	123	CB	THR	B	277	-34.042	83.632	3.048	1.00	44.97	6
	ATOM	124	OG1	THR	B	277	-33.202	84.145	2.001	1.00	46.38	8
	ATOM	125	CG2	THR	B	277	-34.856	84.781	3.653	1.00	37.17	6
30	ATOM	126	C	THR	B	277	-34.069	82.447	5.267	1.00	39.84	6
	ATOM	127	O	THR	B	277	-34.083	83.026	6.375	1.00	40.55	8
	ATOM	128	N	PRO	B	278	-34.832	81.385	5.017	1.00	38.20	7
	ATOM	129	CD	PRO	B	278	-34.925	80.666	3.747	1.00	36.34	6
	ATOM	130	CA	PRO	B	278	-35.711	80.834	6.059	1.00	36.63	6
35	ATOM	131	CB	PRO	B	278	-36.475	79.715	5.357	1.00	32.95	6
	ATOM	132	CG	PRO	B	278	-35.833	79.516	4.056	1.00	35.75	6
	ATOM	133	C	PRO	B	278	-34.892	80.324	7.220	1.00	38.60	6
	ATOM	134	O	PRO	B	278	-35.372	80.157	8.331	1.00	37.67	8
	ATOM	135	N	ALA	B	279	-33.636	80.040	6.927	1.00	37.05	7
40	ATOM	136	CA	ALA	B	279	-32.696	79.525	7.903	1.00	33.18	6
	ATOM	137	CB	ALA	B	279	-31.391	79.195	7.205	1.00	30.56	6
	ATOM	138	C	ALA	B	279	-32.447	80.536	8.991	1.00	33.47	6
	ATOM	139	O	ALA	B	279	-32.623	80.238	10.158	1.00	33.74	8
	ATOM	140	N	ILE	B	280	-32.010	81.728	8.577	1.00	29.96	7
45	ATOM	141	CA	ILE	B	280	-31.728	82.809	9.501	1.00	25.94	6
	ATOM	142	CB	ILE	B	280	-31.190	84.040	8.754	1.00	26.95	6
	ATOM	143	CG2	ILE	B	280	-30.881	85.149	9.715	1.00	15.40	6
	ATOM	144	CG1	ILE	B	280	-29.904	83.696	8.007	1.00	26.73	6
	ATOM	145	CD1	ILE	B	280	-29.255	84.878	7.362	1.00	34.31	6
50	ATOM	146	C	ILE	B	280	-32.964	83.172	10.310	1.00	31.39	6
	ATOM	147	O	ILE	B	280	-32.882	83.378	11.522	1.00	35.69	8
	ATOM	148	N	THR	B	281	-34.113	83.233	9.647	1.00	30.90	7
	ATOM	149	CA	THR	B	281	-35.361	83.586	10.328	1.00	33.49	6
	ATOM	150	CB	THR	B	281	-36.598	83.396	9.419	1.00	37.18	6
55	ATOM	151	OG1	THR	B	281	-36.703	82.034	9.005	1.00	46.48	8
	ATOM	152	CG2	THR	B	281	-36.525	84.289	8.198	1.00	32.85	6
	ATOM	153	C	THR	B	281	-35.523	82.706	11.556	1.00	29.94	6
	ATOM	154	O	THR	B	281	-35.855	83.186	12.634	1.00	25.55	8

5	ATOM	155	N	ARG	B	282	-35.296	81.405	11.378	1.00	32.70	7
	ATOM	156	CA	ARG	B	282	-35.439	80.449	12.475	1.00	34.27	6
	ATOM	157	CB	ARG	B	282	-34.999	79.060	12.020	1.00	33.78	6
	ATOM	158	CG	ARG	B	282	-35.986	77.944	12.280	1.00	45.15	6
	ATOM	159	CD	ARG	B	282	-36.701	77.514	11.015	1.00	58.24	6
10	ATOM	160	NE	ARG	B	282	-35.771	77.153	9.969	1.00	68.41	7
	ATOM	161	CZ	ARG	B	282	-34.862	76.200	10.098	1.00	72.31	6
	ATOM	162	NH1	ARG	B	282	-34.779	75.502	11.232	1.00	77.89	7
	ATOM	163	NH2	ARG	B	282	-34.022	75.963	9.096	1.00	69.25	7
	ATOM	164	C	ARG	B	282	-34.556	80.919	13.622	1.00	34.81	6
15	ATOM	165	O	ARG	B	282	-35.008	81.034	14.753	1.00	36.03	8
	ATOM	166	N	VAL	B	283	-33.288	81.183	13.289	1.00	31.71	7
	ATOM	167	CA	VAL	B	283	-32.304	81.667	14.249	1.00	30.16	6
	ATOM	168	CB	VAL	B	283	-30.993	82.029	13.559	1.00	29.00	6
	ATOM	169	CG1	VAL	B	283	-30.015	82.617	14.557	1.00	28.64	6
20	ATOM	170	CG2	VAL	B	283	-30.385	80.816	12.915	1.00	28.28	6
	ATOM	171	C	VAL	B	283	-32.848	82.884	14.994	1.00	32.50	6
	ATOM	172	O	VAL	B	283	-32.619	83.057	16.185	1.00	33.48	8
	ATOM	173	N	VAL	B	284	-33.573	83.728	14.265	1.00	30.96	7
	ATOM	174	CA	VAL	B	284	-34.177	84.925	14.844	1.00	29.14	6
25	ATOM	175	CB	VAL	B	284	-34.672	85.892	13.751	1.00	31.27	6
	ATOM	176	CG1	VAL	B	284	-35.278	87.129	14.371	1.00	24.21	6
	ATOM	177	CG2	VAL	B	284	-33.554	86.270	12.812	1.00	30.51	6
	ATOM	178	C	VAL	B	284	-35.336	84.498	15.747	1.00	28.89	6
	ATOM	179	O	VAL	B	284	-35.491	84.994	16.860	1.00	27.29	8
30	ATOM	180	N	ASP	B	285	-36.143	83.564	15.250	1.00	28.76	7
	ATOM	181	CA	ASP	B	285	-37.299	83.057	15.983	1.00	35.32	6
	ATOM	182	CB	ASP	B	285	-38.129	82.098	15.111	1.00	33.29	6
	ATOM	183	CG	ASP	B	285	-38.881	82.795	14.013	1.00	38.15	6
	ATOM	184	OD1	ASP	B	285	-39.660	83.729	14.305	1.00	34.70	8
35	ATOM	185	OD2	ASP	B	285	-38.741	82.406	12.821	1.00	34.43	8
	ATOM	186	C	ASP	B	285	-36.863	82.339	17.257	1.00	36.70	6
	ATOM	187	O	ASP	B	285	-37.606	82.304	18.237	1.00	37.96	8
	ATOM	188	N	PHE	B	286	-35.663	81.755	17.235	1.00	35.96	7
	ATOM	189	CA	PHE	B	286	-35.134	81.053	18.401	1.00	37.10	6
40	ATOM	190	CB	PHE	B	286	-33.870	80.262	18.052	1.00	37.97	6
	ATOM	191	CG	PHE	B	286	-33.079	79.818	19.258	1.00	36.50	6
	ATOM	192	CD1	PHE	B	286	-33.704	79.168	20.294	1.00	36.75	6
	ATOM	193	CD2	PHE	B	286	-31.721	80.063	19.343	1.00	33.83	6
	ATOM	194	CE1	PHE	B	286	-32.987	78.769	21.401	1.00	39.55	6
45	ATOM	195	CE2	PHE	B	286	-30.997	79.662	20.456	1.00	38.08	6
	ATOM	196	CZ	PHE	B	286	-31.632	79.013	21.486	1.00	34.44	6
	ATOM	197	C	PHE	B	286	-34.808	82.023	19.504	1.00	36.83	6
	ATOM	198	O	PHE	B	286	-35.246	81.845	20.631	1.00	35.61	8
	ATOM	199	N	ALA	B	287	-34.005	83.027	19.169	1.00	37.33	7
50	ATOM	200	CA	ALA	B	287	-33.599	84.035	20.132	1.00	36.34	6
	ATOM	201	CB	ALA	B	287	-32.644	85.008	19.469	1.00	36.40	6
	ATOM	202	C	ALA	B	287	-34.831	84.769	20.657	1.00	38.76	6
	ATOM	203	O	ALA	B	287	-34.882	85.193	21.814	1.00	41.98	8
	ATOM	204	N	LYS	B	288	-35.820	84.912	19.779	1.00	38.28	7
55	ATOM	205	CA	LYS	B	288	-37.066	85.584	20.112	1.00	45.26	6
	ATOM	206	CB	LYS	B	288	-37.983	85.690	18.898	1.00	48.35	6
	ATOM	207	CG	LYS	B	288	-37.577	86.756	17.916	1.00	51.43	6
	ATOM	208	CD	LYS	B	288	-38.806	87.359	17.226	1.00	60.23	6

5	ATOM	209	CE	LYS	B	288	-39.680	86.308	16.564	1.00	62.81	6
	ATOM	210	NZ	LYS	B	288	-38.897	85.460	15.614	1.00	64.69	7
	ATOM	211	C	LYS	B	288	-37.846	84.901	21.191	1.00	43.31	6
	ATOM	212	O	LYS	B	288	-38.650	85.532	21.857	1.00	45.66	8
	ATOM	213	N	LYS	B	289	-37.618	83.604	21.345	1.00	41.70	7
10	ATOM	214	CA	LYS	B	289	-38.313	82.849	22.351	1.00	40.67	6
	ATOM	215	CB	LYS	B	289	-38.554	81.418	21.845	1.00	42.25	6
	ATOM	216	CG	LYS	B	289	-39.438	81.368	20.589	1.00	39.53	6
	ATOM	217	CD	LYS	B	289	-40.093	80.010	20.422	1.00	43.19	6
	ATOM	218	CE	LYS	B	289	-41.025	79.987	19.223	1.00	45.74	6
15	ATOM	219	NZ	LYS	B	289	-42.391	80.476	19.512	1.00	52.49	7
	ATOM	220	C	LYS	B	289	-37.555	82.871	23.668	1.00	41.50	6
	ATOM	221	O	LYS	B	289	-38.057	82.366	24.657	1.00	39.77	8
	ATOM	222	N	LEU	B	290	-36.365	83.482	23.661	1.00	40.68	7
	ATOM	223	CA	LEU	B	290	-35.539	83.599	24.854	1.00	39.33	6
20	ATOM	224	CB	LEU	B	290	-34.053	83.499	24.491	1.00	36.14	6
	ATOM	225	CG	LEU	B	290	-33.640	82.240	23.767	1.00	34.81	6
	ATOM	226	CD1	LEU	B	290	-32.147	82.255	23.523	1.00	29.07	6
	ATOM	227	CD2	LEU	B	290	-34.013	81.040	24.607	1.00	33.45	6
	ATOM	228	C	LEU	B	290	-35.832	84.915	25.577	1.00	40.08	6
25	ATOM	229	O	LEU	B	290	-35.479	86.006	25.088	1.00	42.00	8
	ATOM	230	N	PRO	B	291	-36.462	84.840	26.765	1.00	40.27	7
	ATOM	231	CD	PRO	B	291	-36.819	83.613	27.494	1.00	39.65	6
	ATOM	232	CA	PRO	B	291	-36.782	86.069	27.501	1.00	38.28	6
	ATOM	233	CB	PRO	B	291	-37.376	85.574	28.811	1.00	35.88	6
30	ATOM	234	CG	PRO	B	291	-37.549	84.110	28.695	1.00	34.19	6
	ATOM	235	C	PRO	B	291	-35.570	87.002	27.714	1.00	40.05	6
	ATOM	236	O	PRO	B	291	-35.625	88.197	27.403	1.00	41.33	8
	ATOM	237	N	MET	B	292	-34.474	86.476	28.258	1.00	40.59	7
	ATOM	238	CA	MET	B	292	-33.296	87.286	28.545	1.00	42.86	6
35	ATOM	239	CB	MET	B	292	-32.149	86.376	28.975	1.00	43.28	6
	ATOM	240	CG	MET	B	292	-32.553	85.302	29.970	1.00	50.35	6
	ATOM	241	SD	MET	B	292	-31.070	84.609	30.755	1.00	51.17	16
	ATOM	242	CE	MET	B	292	-31.797	83.212	31.701	1.00	54.63	6
	ATOM	243	C	MET	B	292	-32.895	88.077	27.315	1.00	41.05	6
40	ATOM	244	O	MET	B	292	-32.228	89.098	27.420	1.00	39.66	8
	ATOM	245	N	PHE	B	293	-33.322	87.604	26.143	1.00	39.30	7
	ATOM	246	CA	PHE	B	293	-33.017	88.271	24.878	1.00	40.92	6
	ATOM	247	CB	PHE	B	293	-33.296	87.329	23.707	1.00	40.98	6
	ATOM	248	CG	PHE	B	293	-32.937	87.909	22.365	1.00	42.78	6
45	ATOM	249	CD1	PHE	B	293	-31.653	88.354	22.120	1.00	44.40	6
	ATOM	250	CD2	PHE	B	293	-33.872	87.972	21.350	1.00	43.66	6
	ATOM	251	CE1	PHE	B	293	-31.306	88.869	20.872	1.00	39.83	6
	ATOM	252	CE2	PHE	B	293	-33.525	88.486	20.100	1.00	46.21	6
	ATOM	253	CZ	PHE	B	293	-32.239	88.926	19.859	1.00	45.18	6
50	ATOM	254	C	PHE	B	293	-33.873	89.518	24.744	1.00	45.54	6
	ATOM	255	O	PHE	B	293	-33.369	90.626	24.579	1.00	42.01	8
	ATOM	256	N	CYS	B	294	-35.181	89.305	24.808	1.00	47.05	7
	ATOM	257	CA	CYS	B	294	-36.146	90.382	24.689	1.00	50.15	6
	ATOM	258	CB	CYS	B	294	-37.553	89.793	24.756	1.00	45.90	6
55	ATOM	259	SG	CYS	B	294	-37.899	88.607	23.449	1.00	51.50	16
	ATOM	260	C	CYS	B	294	-35.974	91.474	25.751	1.00	51.38	6
	ATOM	261	O	CYS	B	294	-36.585	92.536	25.656	1.00	53.83	8
	ATOM	262	N	GLU	B	295	-35.137	91.200	26.753	1.00	49.72	7

5	ATOM	263	CA	GLU B 295	-34.839	92.159	27.816	1.00	52.53	6
	ATOM	264	CB	GLU B 295	-34.553	91.412	29.131	1.00	57.40	6
	ATOM	265	CG	GLU B 295	-35.811	90.978	29.874	1.00	69.63	6
	ATOM	266	CD	GLU B 295	-36.610	92.144	30.375	1.00	78.49	6
	ATOM	267	OE1	GLU B 295	-36.153	92.869	31.297	1.00	82.82	8
10	ATOM	268	OE2	GLU B 295	-37.730	92.385	29.860	1.00	85.30	8
	ATOM	269	C	GLU B 295	-33.629	93.009	27.415	1.00	48.54	6
	ATOM	270	O	GLU B 295	-32.981	93.627	28.260	1.00	49.82	8
	ATOM	271	N	LEU B 296	-33.374	93.030	26.109	1.00	43.79	7
	ATOM	272	CA	LEU B 296	-32.268	93.761	25.540	1.00	45.42	6
15	ATOM	273	CB	LEU B 296	-31.319	92.769	24.838	1.00	41.04	6
	ATOM	274	CG	LEU B 296	-30.735	91.631	25.662	1.00	42.74	6
	ATOM	275	CD1	LEU B 296	-30.354	90.478	24.764	1.00	40.99	6
	ATOM	276	CD2	LEU B 296	-29.559	92.119	26.468	1.00	39.44	6
	ATOM	277	C	LEU B 296	-32.760	94.779	24.522	1.00	45.56	6
20	ATOM	278	O	LEU B 296	-33.845	94.600	23.924	1.00	43.07	8
	ATOM	279	N	PRO B 297	-32.004	95.875	24.338	1.00	46.99	7
	ATOM	280	CD	PRO B 297	-30.740	96.123	25.046	1.00	47.12	6
	ATOM	281	CA	PRO B 297	-32.388	96.912	23.363	1.00	49.61	6
	ATOM	282	CB	PRO B 297	-31.294	97.973	23.494	1.00	49.91	6
25	ATOM	283	CG	PRO B 297	-30.302	97.477	24.545	1.00	51.28	6
	ATOM	284	C	PRO B 297	-32.263	96.273	21.913	1.00	49.59	6
	ATOM	285	O	PRO B 297	-31.441	95.340	21.685	1.00	51.66	8
	ATOM	286	N	CYS B 298	-33.035	96.667	20.854	1.00	51.02	7
	ATOM	287	CA	CYS B 298	-32.761	96.150	19.456	1.00	52.86	6
30	ATOM	288	CB	CYS B 298	-33.140	97.165	18.356	1.00	54.57	6
	ATOM	289	SG	CYS B 298	-34.884	97.085	17.836	1.00	67.87	16
	ATOM	290	C	CYS B 298	-31.385	96.330	19.127	1.00	48.51	6
	ATOM	291	O	CYS B 298	-30.579	95.506	18.744	1.00	49.58	8
	ATOM	292	N	GLU B 299	-31.107	97.447	19.230	1.00	44.17	7
35	ATOM	293	CA	GLU B 299	-29.989	97.645	18.718	1.00	47.57	6
	ATOM	294	CB	GLU B 299	-29.402	98.973	19.208	1.00	49.92	6
	ATOM	295	CG	GLU B 299	-29.944	100.187	18.433	1.00	59.30	6
	ATOM	296	CD	GLU B 299	-31.090	100.887	19.164	1.00	63.80	6
	ATOM	297	OE1	GLU B 299	-31.673	101.904	18.629	1.00	69.03	8
40	ATOM	298	OE2	GLU B 299	-31.473	100.458	20.319	1.00	67.10	8
	ATOM	299	C	GLU B 299	-28.993	96.533	18.987	1.00	46.57	6
	ATOM	300	O	GLU B 299	-28.200	96.179	18.111	1.00	44.65	8
	ATOM	301	N	ASP B 300	-29.045	95.989	20.203	1.00	45.17	7
	ATOM	302	CA	ASP B 300	-28.152	94.908	20.584	1.00	43.32	6
45	ATOM	303	CB	ASP B 300	-27.985	94.849	22.105	1.00	37.38	6
	ATOM	304	CG	ASP B 300	-27.239	96.016	22.650	1.00	36.23	6
	ATOM	305	OD1	ASP B 300	-26.208	96.421	22.052	1.00	35.87	8
	ATOM	306	OD2	ASP B 300	-27.661	96.543	23.716	1.00	40.14	8
	ATOM	307	C	ASP B 300	-28.721	93.591	20.071	1.00	42.81	6
50	ATOM	308	O	ASP B 300	-28.001	92.775	19.489	1.00	46.02	8
	ATOM	309	N	GLN B 301	-30.019	93.399	20.306	1.00	38.60	7
	ATOM	310	CA	GLN B 301	-30.712	92.197	19.858	1.00	40.00	6
	ATOM	311	CB	GLN B 301	-32.234	92.418	19.836	1.00	38.59	6
	ATOM	312	CG	GLN B 301	-32.908	92.380	21.187	1.00	40.26	6
55	ATOM	313	CD	GLN B 301	-34.401	92.583	21.083	1.00	44.15	6
	ATOM	314	OE1	GLN B 301	-34.859	93.637	20.589	1.00	45.73	8
	ATOM	315	NE2	GLN B 301	-35.165	91.602	21.544	1.00	46.13	7
	ATOM	316	C	GLN B 301	-30.237	91.830	18.455	1.00	41.64	6

5	ATOM	317	O	GLN	B	301	-30.162	90.662	18.100	1.00	45.02	8
	ATOM	318	N	ILE	B	302	-29.916	92.864	17.674	1.00	41.01	7
	ATOM	319	CA	ILE	B	302	-29.424	92.692	16.311	1.00	40.23	6
	ATOM	320	CB	ILE	B	302	-29.584	93.978	15.498	1.00	39.52	6
	ATOM	321	CG2	ILE	B	302	-29.034	93.792	14.100	1.00	31.98	6
10	ATOM	322	CG1	ILE	B	302	-31.059	94.385	15.416	1.00	40.77	6
	ATOM	323	CD1	ILE	B	302	-31.939	93.317	14.775	1.00	45.43	6
	ATOM	324	C	ILE	B	302	-27.966	92.260	16.342	1.00	38.58	6
	ATOM	325	O	ILE	B	302	-27.613	91.197	15.830	1.00	40.81	8
	ATOM	326	N	ILE	B	303	-27.128	93.111	16.933	1.00	37.50	7
15	ATOM	327	CA	ILE	B	303	-25.692	92.846	17.062	1.00	39.33	6
	ATOM	328	CB	ILE	B	303	-25.066	93.648	18.203	1.00	39.06	6
	ATOM	329	CG2	ILE	B	303	-23.566	93.405	18.257	1.00	36.19	6
	ATOM	330	CG1	ILE	B	303	-25.309	95.143	18.020	1.00	40.15	6
	ATOM	331	CD1	ILE	B	303	-24.816	95.966	19.173	1.00	36.93	6
20	ATOM	332	C	ILE	B	303	-25.470	91.365	17.323	1.00	36.49	6
	ATOM	333	O	ILE	B	303	-24.619	90.725	16.712	1.00	36.58	8
	ATOM	334	N	LEU	B	304	-26.244	90.843	18.266	1.00	32.91	7
	ATOM	335	CA	LEU	B	304	-26.194	89.433	18.633	1.00	27.55	6
	ATOM	336	CB	LEU	B	304	-27.172	89.182	19.793	1.00	22.35	6
25	ATOM	337	CG	LEU	B	304	-26.623	89.449	21.187	1.00	26.88	6
	ATOM	338	CD1	LEU	B	304	-25.540	90.495	21.136	1.00	24.82	6
	ATOM	339	CD2	LEU	B	304	-27.747	89.840	22.121	1.00	23.69	6
	ATOM	340	C	LEU	B	304	-26.505	88.547	17.425	1.00	28.05	6
	ATOM	341	O	LEU	B	304	-25.668	87.751	16.983	1.00	24.68	8
30	ATOM	342	N	LEU	B	305	-27.716	88.700	16.897	1.00	26.34	7
	ATOM	343	CA	LEU	B	305	-28.145	87.939	15.741	1.00	30.91	6
	ATOM	344	CB	LEU	B	305	-29.460	88.514	15.199	1.00	32.50	6
	ATOM	345	CG	LEU	B	305	-30.699	88.305	16.050	1.00	33.36	6
	ATOM	346	CD1	LEU	B	305	-31.938	88.839	15.342	1.00	33.87	6
35	ATOM	347	CD2	LEU	B	305	-30.863	86.812	16.298	1.00	31.72	6
	ATOM	348	C	LEU	B	305	-27.072	87.922	14.666	1.00	29.76	6
	ATOM	349	O	LEU	B	305	-26.687	86.860	14.202	1.00	29.33	8
	ATOM	350	N	LYS	B	306	-26.597	89.107	14.291	1.00	29.72	7
	ATOM	351	CA	LYS	B	306	-25.576	89.254	13.264	1.00	34.28	6
40	ATOM	352	CB	LYS	B	306	-25.224	90.732	13.077	1.00	35.98	6
	ATOM	353	CG	LYS	B	306	-26.350	91.581	12.494	1.00	43.35	6
	ATOM	354	CD	LYS	B	306	-25.852	92.987	12.182	1.00	51.50	6
	ATOM	355	CE	LYS	B	306	-24.706	92.932	11.190	1.00	53.26	6
	ATOM	356	NZ	LYS	B	306	-23.883	94.161	11.251	1.00	59.61	7
45	ATOM	357	C	LYS	B	306	-24.308	88.484	13.556	1.00	35.25	6
	ATOM	358	O	LYS	B	306	-23.681	87.917	12.653	1.00	33.95	8
	ATOM	359	N	GLY	B	307	-23.918	88.478	14.829	1.00	35.79	7
	ATOM	360	CA	GLY	B	307	-22.702	87.793	15.227	1.00	34.59	6
	ATOM	361	C	GLY	B	307	-22.811	86.291	15.383	1.00	33.80	6
50	ATOM	362	O	GLY	B	307	-21.944	85.564	14.895	1.00	31.59	8
	ATOM	363	N	CYS	B	308	-23.861	85.843	16.071	1.00	31.15	7
	ATOM	364	CA	CYS	B	308	-24.069	84.434	16.320	1.00	29.04	6
	ATOM	365	CB	CYS	B	308	-24.761	84.240	17.663	1.00	27.59	6
	ATOM	366	SG	CYS	B	308	-26.496	84.629	17.608	1.00	30.50	16
55	ATOM	367	C	CYS	B	308	-24.911	83.712	15.266	1.00	30.59	6
	ATOM	368	O	CYS	B	308	-25.088	82.499	15.365	1.00	33.77	8
	ATOM	369	N	CYS	B	309	-25.432	84.429	14.266	1.00	28.46	7
	ATOM	370	CA	CYS	B	309	-26.270	83.787	13.265	1.00	30.10	6

5	ATOM	371	CB	CYS B 309	-26.706	84.761	12.194	1.00	33.43	6
	ATOM	372	SG	CYS B 309	-27.875	84.011	11.089	1.00	35.20	16
	ATOM	373	C	CYS B 309	-25.617	82.608	12.603	1.00	27.72	6
	ATOM	374	O	CYS B 309	-26.170	81.518	12.610	1.00	27.69	8
	ATOM	375	N	MET B 310	-24.447	82.829	12.011	1.00	26.15	7
10	ATOM	376	CA	MET B 310	-23.737	81.748	11.352	1.00	26.06	6
	ATOM	377	CB	MET B 310	-22.439	82.263	10.712	1.00	25.32	6
	ATOM	378	CG	MET B 310	-21.584	81.157	10.080	1.00	24.08	6
	ATOM	379	SD	MET B 310	-22.555	80.324	8.758	1.00	27.71	16
	ATOM	380	CE	MET B 310	-21.549	78.826	8.427	1.00	28.50	6
15	ATOM	381	C	MET B 310	-23.416	80.673	12.374	1.00	25.94	6
	ATOM	382	O	MET B 310	-23.659	79.489	12.151	1.00	28.09	8
	ATOM	383	N	GLU B 311	-22.865	81.117	13.500	1.00	25.39	7
	ATOM	384	CA	GLU B 311	-22.466	80.231	14.576	1.00	27.03	6
	ATOM	385	CB	GLU B 311	-22.036	81.048	15.797	1.00	24.39	6
20	ATOM	386	CG	GLU B 311	-21.019	82.141	15.509	1.00	26.00	6
	ATOM	387	CD	GLU B 311	-20.524	82.835	16.740	1.00	23.95	6
	ATOM	388	OE1	GLU B 311	-21.321	83.108	17.668	1.00	19.72	8
	ATOM	389	OE2	GLU B 311	-19.313	83.163	16.815	1.00	26.51	8
	ATOM	390	C	GLU B 311	-23.582	79.264	14.964	1.00	27.51	6
25	ATOM	391	O	GLU B 311	-23.347	78.068	15.093	1.00	29.67	8
	ATOM	392	N	ILE B 312	-24.794	79.792	15.145	1.00	26.82	7
	ATOM	393	CA	ILE B 312	-25.933	78.967	15.527	1.00	25.71	6
	ATOM	394	CB	ILE B 312	-27.125	79.814	16.021	1.00	23.35	6
	ATOM	395	CG2	ILE B 312	-28.327	78.933	16.276	1.00	20.27	6
30	ATOM	396	CG1	ILE B 312	-26.771	80.541	17.325	1.00	20.88	6
	ATOM	397	CD1	ILE B 312	-27.952	81.163	18.028	1.00	18.15	6
	ATOM	398	C	ILE B 312	-26.370	78.072	14.392	1.00	27.91	6
	ATOM	399	O	ILE B 312	-26.769	76.926	14.605	1.00	28.96	8
	ATOM	400	N	MET B 313	-26.303	78.603	13.174	1.00	27.66	7
35	ATOM	401	CA	MET B 313	-26.696	77.832	11.999	1.00	30.18	6
	ATOM	402	CB	MET B 313	-26.696	78.691	10.734	1.00	36.89	6
	ATOM	403	CG	MET B 313	-27.882	79.634	10.607	1.00	37.95	6
	ATOM	404	SD	MET B 313	-28.238	80.275	8.907	1.00	42.38	16
	ATOM	405	CE	MET B 313	-26.787	81.316	8.639	1.00	40.68	6
40	ATOM	406	C	MET B 313	-25.791	76.632	11.808	1.00	27.43	6
	ATOM	407	O	MET B 313	-26.258	75.501	11.893	1.00	28.61	8
	ATOM	408	N	SER B 314	-24.508	76.882	11.549	1.00	24.88	7
	ATOM	409	CA	SER B 314	-23.533	75.824	11.346	1.00	27.98	6
	ATOM	410	CB	SER B 314	-22.150	76.441	11.165	1.00	29.64	6
45	ATOM	411	OG	SER B 314	-21.844	77.316	12.227	1.00	43.44	8
	ATOM	412	C	SER B 314	-23.514	74.774	12.465	1.00	22.30	6
	ATOM	413	O	SER B 314	-23.279	73.592	12.199	1.00	24.18	8
	ATOM	414	N	LEU B 315	-23.760	75.187	13.714	1.00	23.99	7
	ATOM	415	CA	LEU B 315	-23.792	74.219	14.811	1.00	25.07	6
50	ATOM	416	CB	LEU B 315	-24.095	74.869	16.169	1.00	19.11	6
	ATOM	417	CG	LEU B 315	-24.507	73.860	17.234	1.00	20.39	6
	ATOM	418	CD1	LEU B 315	-23.390	72.878	17.493	1.00	18.92	6
	ATOM	419	CD2	LEU B 315	-24.895	74.560	18.514	1.00	12.93	6
	ATOM	420	C	LEU B 315	-24.892	73.219	14.517	1.00	24.53	6
55	ATOM	421	O	LEU B 315	-24.672	72.014	14.550	1.00	26.32	8
	ATOM	422	N	ARG B 316	-26.079	73.762	14.254	1.00	28.18	7
	ATOM	423	CA	ARG B 316	-27.278	72.996	13.971	1.00	27.54	6
	ATOM	424	CB	ARG B 316	-28.432	73.941	13.651	1.00	27.39	6



5	ATOM	425	CG	ARG B 316	-28.823	74.857	14.809	1.00	22.00	6
	ATOM	426	CD	ARG B 316	-30.074	75.657	14.451	1.00	18.78	6
	ATOM	427	NE	ARG B 316	-30.905	75.944	15.598	1.00	26.57	7
	ATOM	428	CZ	ARG B 316	-32.166	76.337	15.489	1.00	30.81	6
	ATOM	429	NH1	ARG B 316	-32.686	76.535	14.280	1.00	33.71	7
10	ATOM	430	NH2	ARG B 316	-32.900	76.542	16.581	1.00	33.13	7
	ATOM	431	C	ARG B 316	-27.128	72.028	12.830	1.00	28.09	6
	ATOM	432	O	ARG B 316	-27.852	71.053	12.760	1.00	32.41	8
	ATOM	433	N	ALA B 317	-26.187	72.309	11.941	1.00	28.36	7
	ATOM	434	CA	ALA B 317	-25.938	71.466	10.794	1.00	26.64	6
15	ATOM	435	CB	ALA B 317	-25.337	72.300	9.675	1.00	22.93	6
	ATOM	436	C	ALA B 317	-24.998	70.327	11.150	1.00	28.35	6
	ATOM	437	O	ALA B 317	-25.223	69.187	10.773	1.00	32.10	8
	ATOM	438	N	ALA B 318	-23.941	70.659	11.882	1.00	29.12	7
	ATOM	439	CA	ALA B 318	-22.957	69.682	12.299	1.00	27.50	6
20	ATOM	440	CB	ALA B 318	-21.915	70.355	13.160	1.00	28.39	6
	ATOM	441	C	ALA B 318	-23.645	68.591	13.084	1.00	28.10	6
	ATOM	442	O	ALA B 318	-23.415	67.415	12.854	1.00	28.18	8
	ATOM	443	N	VAL B 319	-24.502	69.012	14.016	1.00	29.16	7
	ATOM	444	CA	VAL B 319	-25.259	68.107	14.889	1.00	35.24	6
25	ATOM	445	CB	VAL B 319	-26.228	68.897	15.765	1.00	27.34	6
	ATOM	446	CG1	VAL B 319	-25.576	70.149	16.246	1.00	29.96	6
	ATOM	447	CG2	VAL B 319	-27.505	69.212	15.022	1.00	31.70	6
	ATOM	448	C	VAL B 319	-26.066	67.146	14.043	1.00	40.01	6
	ATOM	449	O	VAL B 319	-26.701	66.250	14.578	1.00	42.70	8
30	ATOM	450	N	ARG B 320	-26.025	67.353	12.723	1.00	38.64	7
	ATOM	451	CA	ARG B 320	-26.770	66.541	11.762	1.00	38.61	6
	ATOM	452	CB	ARG B 320	-27.838	67.409	11.123	1.00	37.26	6
	ATOM	453	CG	ARG B 320	-29.152	67.280	11.822	1.00	43.12	6
	ATOM	454	CD	ARG B 320	-30.145	68.340	11.387	1.00	50.79	6
35	ATOM	455	NE	ARG B 320	-31.500	67.911	11.705	1.00	54.71	7
	ATOM	456	CZ	ARG B 320	-32.555	68.723	11.597	1.00	57.89	6
	ATOM	457	NH1	ARG B 320	-32.398	69.957	11.130	1.00	49.08	7
	ATOM	458	NH2	ARG B 320	-33.773	68.302	11.844	1.00	59.59	7
	ATOM	459	C	ARG B 320	-25.937	65.910	10.670	1.00	42.14	6
40	ATOM	460	O	ARG B 320	-26.381	65.802	9.532	1.00	46.30	8
	ATOM	461	N	TYR B 321	-24.734	65.488	11.022	1.00	42.04	7
	ATOM	462	CA	TYR B 321	-23.858	64.848	10.063	1.00	42.70	6
	ATOM	463	CB	TYR B 321	-22.433	65.332	10.297	1.00	38.01	6
	ATOM	464	CG	TYR B 321	-21.393	64.396	9.756	1.00	37.94	6
45	ATOM	465	CD1	TYR B 321	-21.265	64.176	8.397	1.00	33.85	6
	ATOM	466	CE1	TYR B 321	-20.333	63.258	7.912	1.00	34.49	6
	ATOM	467	CD2	TYR B 321	-20.583	63.683	10.613	1.00	28.03	6
	ATOM	468	CE2	TYR B 321	-19.658	62.769	10.134	1.00	32.69	6
	ATOM	469	CZ	TYR B 321	-19.532	62.551	8.781	1.00	35.18	6
50	ATOM	470	OH	TYR B 321	-18.616	61.661	8.292	1.00	39.48	8
	ATOM	471	C	TYR B 321	-23.897	63.347	10.234	1.00	45.51	6
	ATOM	472	O	TYR B 321	-23.560	62.857	11.292	1.00	48.02	8
	ATOM	473	N	ASP B 322	-24.317	62.642	9.188	1.00	44.56	7
	ATOM	474	CA	ASP B 322	-24.391	61.170	9.182	1.00	45.86	6
55	ATOM	475	CB	ASP B 322	-25.570	60.749	8.294	1.00	46.64	6
	ATOM	476	CG	ASP B 322	-25.449	59.359	7.775	1.00	40.00	6
	ATOM	477	OD1	ASP B 322	-24.388	58.737	7.986	1.00	40.00	8
	ATOM	478	OD2	ASP B 322	-26.414	58.862	7.117	1.00	40.00	8

5	ATOM	479	C	ASP	B	322	-23.044	60.659	8.682	1.00	45.82	6
	ATOM	480	O	ASP	B	322	-22.738	60.783	7.495	1.00	45.38	8
	ATOM	481	N	PRO	B	323	-22.242	60.005	9.549	1.00	46.53	7
	ATOM	482	CD	PRO	B	323	-22.594	59.676	10.934	1.00	47.16	6
	ATOM	483	CA	PRO	B	323	-20.910	59.487	9.162	1.00	46.63	6
10	ATOM	484	CB	PRO	B	323	-20.367	58.847	10.433	1.00	43.95	6
	ATOM	485	CG	PRO	B	323	-21.398	58.958	11.454	1.00	43.93	6
	ATOM	486	C	PRO	B	323	-20.933	58.489	8.017	1.00	48.34	6
	ATOM	487	O	PRO	B	323	-20.040	58.457	7.171	1.00	50.84	8
	ATOM	488	N	GLU	B	324	-21.951	57.631	8.022	1.00	52.39	7
15	ATOM	489	CA	GLU	B	324	-22.126	56.615	7.008	1.00	55.85	6
	ATOM	490	CB	GLU	B	324	-23.491	55.960	7.216	1.00	55.54	6
	ATOM	491	CG	GLU	B	324	-23.678	55.332	8.581	1.00	40.00	6
	ATOM	492	CD	GLU	B	324	-22.642	54.294	8.888	1.00	40.00	6
	ATOM	493	OE1	GLU	B	324	-21.796	53.979	8.000	1.00	40.00	8
20	ATOM	494	OE2	GLU	B	324	-22.645	53.751	10.029	1.00	40.00	8
	ATOM	495	C	GLU	B	324	-22.087	57.292	5.655	1.00	54.94	6
	ATOM	496	O	GLU	B	324	-21.144	57.149	4.896	1.00	59.81	8
	ATOM	497	N	SER	B	325	-23.165	58.022	5.389	1.00	52.95	7
	ATOM	498	CA	SER	B	325	-23.358	58.762	4.163	1.00	50.10	6
25	ATOM	499	CB	SER	B	325	-24.768	59.357	4.163	1.00	48.23	6
	ATOM	500	OG	SER	B	325	-25.051	59.976	5.403	1.00	48.71	8
	ATOM	501	C	SER	B	325	-22.324	59.861	3.964	1.00	50.61	6
	ATOM	502	O	SER	B	325	-21.956	60.176	2.848	1.00	52.19	8
	ATOM	503	N	GLU	B	326	-21.851	60.422	5.070	1.00	45.64	7
30	ATOM	504	CA	GLU	B	326	-20.854	61.476	5.050	1.00	43.35	6
	ATOM	505	CB	GLU	B	326	-19.602	61.022	4.277	1.00	42.74	6
	ATOM	506	CG	GLU	B	326	-18.880	59.814	4.876	1.00	50.32	6
	ATOM	507	CD	GLU	B	326	-17.576	59.524	4.207	1.00	56.34	6
	ATOM	508	OE1	GLU	B	326	-16.898	58.545	4.608	1.00	59.31	8
35	ATOM	509	OE2	GLU	B	326	-17.177	60.255	3.266	1.00	55.74	8
	ATOM	510	C	GLU	B	326	-21.401	62.731	4.418	1.00	40.23	6
	ATOM	511	O	GLU	B	326	-20.793	63.285	3.514	1.00	40.44	8
	ATOM	512	N	THR	B	327	-22.528	63.208	4.934	1.00	35.90	7
	ATOM	513	CA	THR	B	327	-23.163	64.418	4.401	1.00	37.29	6
40	ATOM	514	CB	THR	B	327	-24.146	64.052	3.285	1.00	37.63	6
	ATOM	515	OG1	THR	B	327	-25.172	63.199	3.803	1.00	38.12	8
	ATOM	516	CG2	THR	B	327	-23.445	63.342	2.130	1.00	39.90	6
	ATOM	517	C	THR	B	327	-23.961	65.125	5.473	1.00	39.49	6
	ATOM	518	O	THR	B	327	-24.645	64.473	6.264	1.00	40.50	8
45	ATOM	519	N	LEU	B	328	-23.909	66.454	5.473	1.00	36.64	7
	ATOM	520	CA	LEU	B	328	-24.675	67.239	6.447	1.00	37.73	6
	ATOM	521	CB	LEU	B	328	-24.061	68.637	6.620	1.00	37.78	6
	ATOM	522	CG	LEU	B	328	-22.586	68.750	6.931	1.00	36.26	6
	ATOM	523	CD1	LEU	B	328	-22.260	70.145	7.411	1.00	36.56	6
50	ATOM	524	CD2	LEU	B	328	-22.231	67.751	8.000	1.00	39.85	6
	ATOM	525	C	LEU	B	328	-26.090	67.344	5.897	1.00	37.27	6
	ATOM	526	O	LEU	B	328	-26.358	66.855	4.805	1.00	34.96	8
	ATOM	527	N	THR	B	329	-26.989	67.975	6.647	1.00	39.73	7
	ATOM	528	CA	THR	B	329	-28.369	68.132	6.215	1.00	40.81	6
55	ATOM	529	CB	THR	B	329	-29.279	67.135	6.918	1.00	42.67	6
	ATOM	530	OG1	THR	B	329	-28.799	65.809	6.686	1.00	42.52	8
	ATOM	531	CG2	THR	B	329	-30.702	67.255	6.375	1.00	43.52	6
	ATOM	532	C	THR	B	329	-28.853	69.529	6.498	1.00	44.31	6

5	ATOM	533	O	THR B 329	-29.432	69.801	7.535	1.00	43.72	8
	ATOM	534	N	LEU B 330	-28.589	70.413	5.546	1.00	44.62	7
	ATOM	535	CA	LEU B 330	-28.983	71.812	5.658	1.00	45.09	6
	ATOM	536	CB	LEU B 330	-28.354	72.608	4.510	1.00	44.66	6
	ATOM	537	CG	LEU B 330	-26.847	72.735	4.539	1.00	51.06	6
10	ATOM	538	CD1	LEU B 330	-26.226	71.367	4.640	1.00	48.58	6
	ATOM	539	CD2	LEU B 330	-26.364	73.450	3.299	1.00	45.18	6
	ATOM	540	C	LEU B 330	-30.508	71.965	5.652	1.00	48.06	6
	ATOM	541	O	LEU B 330	-31.211	71.244	4.959	1.00	49.33	8
	ATOM	542	N	ASN B 331	-30.988	72.911	6.458	1.00	52.20	7
15	ATOM	543	CA	ASN B 331	-32.407	73.214	6.588	1.00	54.41	6
	ATOM	544	CB	ASN B 331	-32.870	74.013	5.370	1.00	54.94	6
	ATOM	545	CG	ASN B 331	-33.687	75.220	5.749	1.00	60.35	6
	ATOM	546	OD1	ASN B 331	-33.182	76.130	6.430	1.00	61.84	8
	ATOM	547	ND2	ASN B 331	-34.935	75.242	5.324	1.00	65.92	7
20	ATOM	548	C	ASN B 331	-33.251	71.959	6.731	1.00	58.00	6
	ATOM	549	O	ASN B 331	-34.464	72.000	6.579	1.00	60.17	8
	ATOM	550	N	GLY B 332	-32.596	70.846	7.054	1.00	58.45	7
	ATOM	551	CA	GLY B 332	-33.295	69.587	7.235	1.00	58.55	6
	ATOM	552	C	GLY B 332	-33.909	69.004	5.984	1.00	59.79	6
25	ATOM	553	O	GLY B 332	-34.609	68.000	6.065	1.00	61.32	8
	ATOM	554	N	GLU B 333	-33.639	69.628	4.838	1.00	60.28	7
	ATOM	555	CA	GLU B 333	-34.196	69.182	3.571	1.00	59.13	6
	ATOM	556	CB	GLU B 333	-34.966	70.323	2.885	1.00	62.40	6
	ATOM	557	CG	GLU B 333	-36.099	70.963	3.690	1.00	75.69	6
30	ATOM	558	CD	GLU B 333	-36.720	72.135	2.998	1.00	80.41	6
	ATOM	559	OE1	GLU B 333	-35.984	73.081	2.618	1.00	79.98	8
	ATOM	560	OE2	GLU B 333	-37.966	72.158	2.830	1.00	83.81	8
	ATOM	561	C	GLU B 333	-33.110	68.722	2.624	1.00	57.18	6
	ATOM	562	O	GLU B 333	-33.236	67.689	1.974	1.00	57.50	8
35	ATOM	563	N	MET B 334	-32.054	69.528	2.539	1.00	55.20	7
	ATOM	564	CA	MET B 334	-30.926	69.259	1.653	1.00	50.85	6
	ATOM	565	CB	MET B 334	-30.514	70.563	0.984	1.00	48.70	6
	ATOM	566	CG	MET B 334	-29.244	70.460	0.194	1.00	45.39	6
	ATOM	567	SD	MET B 334	-28.743	72.008	-0.624	1.00	44.56	16
40	ATOM	568	CE	MET B 334	-30.307	72.445	-1.503	1.00	45.25	6
	ATOM	569	C	MET B 334	-29.711	68.634	2.319	1.00	51.59	6
	ATOM	570	O	MET B 334	-29.185	69.161	3.291	1.00	52.52	8
	ATOM	571	N	ALA B 335	-29.270	67.515	1.758	1.00	51.00	7
	ATOM	572	CA	ALA B 335	-28.106	66.802	2.267	1.00	48.98	6
45	ATOM	573	CB	ALA B 335	-28.377	65.304	2.274	1.00	47.86	6
	ATOM	574	C	ALA B 335	-26.931	67.108	1.371	1.00	51.01	6
	ATOM	575	O	ALA B 335	-26.936	66.760	0.190	1.00	51.61	8
	ATOM	576	N	VAL B 336	-25.921	67.770	1.930	1.00	46.62	7
	ATOM	577	CA	VAL B 336	-24.730	68.142	1.152	1.00	42.35	6
50	ATOM	578	CB	VAL B 336	-24.466	69.635	1.258	1.00	42.41	6
	ATOM	579	CG1	VAL B 336	-25.695	70.418	0.860	1.00	42.00	6
	ATOM	580	CG2	VAL B 336	-24.018	70.004	2.642	1.00	40.32	6
	ATOM	581	C	VAL B 336	-23.493	67.390	1.611	1.00	45.33	6
	ATOM	582	O	VAL B 336	-23.464	66.775	2.681	1.00	47.42	8
55	ATOM	583	N	THR B 337	-22.461	67.478	0.781	1.00	41.60	7
	ATOM	584	CA	THR B 337	-21.172	66.818	1.041	1.00	39.69	6
	ATOM	585	CB	THR B 337	-20.720	66.011	-0.173	1.00	41.35	6
	ATOM	586	OG1	THR B 337	-20.273	66.887	-1.213	1.00	49.35	8

5	ATOM	587	CG2	THR	B	337	-21.869	65.175	-0.702	1.00	40.38	6
	ATOM	588	C	THR	B	337	-20.087	67.846	1.318	1.00	37.88	6
	ATOM	589	O	THR	B	337	-20.141	68.975	0.832	1.00	34.06	8
	ATOM	590	N	ARG	B	338	-19.097	67.417	2.095	1.00	37.61	7
	ATOM	591	CA	ARG	B	338	-17.942	68.241	2.442	1.00	38.68	6
10	ATOM	592	CB	ARG	B	338	-16.770	67.333	2.823	1.00	35.95	6
	ATOM	593	CG	ARG	B	338	-15.455	68.042	3.064	1.00	38.83	6
	ATOM	594	CD	ARG	B	338	-14.348	67.029	3.319	1.00	35.88	6
	ATOM	595	NE	ARG	B	338	-14.520	66.239	4.530	1.00	37.42	7
	ATOM	596	CZ	ARG	B	338	-14.274	66.669	5.766	1.00	30.20	6
15	ATOM	597	NH1	ARG	B	338	-13.794	67.892	5.973	1.00	27.98	7
	ATOM	598	NH2	ARG	B	338	-14.481	65.847	6.788	1.00	27.40	7
	ATOM	599	C	ARG	B	338	-17.581	69.075	1.229	1.00	38.09	6
	ATOM	600	O	ARG	B	338	-17.537	70.299	1.284	1.00	34.12	8
	ATOM	601	N	GLY	B	339	-17.345	68.383	0.117	1.00	41.25	7
20	ATOM	602	CA	GLY	B	339	-16.981	69.054	-1.119	1.00	41.35	6
	ATOM	603	C	GLY	B	339	-18.004	70.109	-1.460	1.00	41.23	6
	ATOM	604	O	GLY	B	339	-17.736	71.291	-1.330	1.00	38.30	8
	ATOM	605	N	GLN	B	340	-19.174	69.665	-1.909	1.00	38.58	7
	ATOM	606	CA	GLN	B	340	-20.258	70.564	-2.276	1.00	40.79	6
25	ATOM	607	CB	GLN	B	340	-21.596	69.843	-2.079	1.00	40.82	6
	ATOM	608	CG	GLN	B	340	-21.830	68.657	-3.029	1.00	41.10	6
	ATOM	609	CD	GLN	B	340	-23.154	67.937	-2.783	1.00	48.84	6
	ATOM	610	OE1	GLN	B	340	-23.353	67.313	-1.715	1.00	50.53	8
	ATOM	611	NE2	GLN	B	340	-24.050	68.015	-3.753	1.00	54.25	7
30	ATOM	612	C	GLN	B	340	-20.239	71.872	-1.475	1.00	41.50	6
	ATOM	613	O	GLN	B	340	-20.114	72.958	-2.032	1.00	42.72	8
	ATOM	614	N	LEU	B	341	-20.352	71.736	-0.156	1.00	42.00	7
	ATOM	615	CA	LEU	B	341	-20.375	72.879	0.746	1.00	38.10	6
	ATOM	616	CB	LEU	B	341	-20.401	72.419	2.201	1.00	36.66	6
35	ATOM	617	CG	LEU	B	341	-20.678	73.514	3.194	1.00	39.94	6
	ATOM	618	CD1	LEU	B	341	-22.088	74.038	2.936	1.00	34.98	6
	ATOM	619	CD2	LEU	B	341	-20.570	72.990	4.609	1.00	40.95	6
	ATOM	620	C	LEU	B	341	-19.170	73.763	0.543	1.00	36.37	6
	ATOM	621	O	LEU	B	341	-19.293	74.974	0.497	1.00	37.89	8
40	ATOM	622	N	LYS	B	342	-18.003	73.136	0.433	1.00	33.29	7
	ATOM	623	CA	LYS	B	342	-16.737	73.843	0.239	1.00	35.17	6
	ATOM	624	CB	LYS	B	342	-15.603	72.821	0.176	1.00	34.97	6
	ATOM	625	CG	LYS	B	342	-14.210	73.401	0.306	1.00	40.00	6
	ATOM	626	CD	LYS	B	342	-13.155	72.288	0.316	1.00	34.48	6
45	ATOM	627	CE	LYS	B	342	-11.775	72.809	0.755	1.00	37.54	6
	ATOM	628	NZ	LYS	B	342	-10.790	71.680	0.981	1.00	42.32	7
	ATOM	629	C	LYS	B	342	-16.744	74.685	-1.038	1.00	38.29	6
	ATOM	630	O	LYS	B	342	-16.725	75.911	-0.993	1.00	36.23	8
	ATOM	631	N	ASN	B	343	-16.760	73.990	-2.172	1.00	39.25	7
50	ATOM	632	CA	ASN	B	343	-16.762	74.609	-3.481	1.00	40.19	6
	ATOM	633	CB	ASN	B	343	-16.977	73.539	-4.551	1.00	37.96	6
	ATOM	634	CG	ASN	B	343	-16.178	72.272	-4.277	1.00	39.22	6
	ATOM	635	OD1	ASN	B	343	-14.938	72.313	-4.106	1.00	42.37	8
	ATOM	636	ND2	ASN	B	343	-16.877	71.144	-4.259	1.00	42.19	7
55	ATOM	637	C	ASN	B	343	-17.894	75.624	-3.547	1.00	40.12	6
	ATOM	638	O	ASN	B	343	-17.835	76.600	-4.284	1.00	36.01	8
	ATOM	639	N	GLY	B	344	-18.934	75.361	-2.756	1.00	40.95	7
	ATOM	640	CA	GLY	B	344	-20.101	76.222	-2.709	1.00	39.25	6

5	ATOM	641	C	GLY	B	344	-19.867	77.636	-2.258	1.00	38.26	6
	ATOM	642	O	GLY	B	344	-20.715	78.501	-2.484	1.00	35.69	8
	ATOM	643	N	GLY	B	345	-18.724	77.871	-1.619	1.00	35.89	7
	ATOM	644	CA	GLY	B	345	-18.426	79.209	-1.159	1.00	34.00	6
	ATOM	645	C	GLY	B	345	-17.848	79.298	0.230	1.00	38.64	6
10	ATOM	646	O	GLY	B	345	-17.216	80.303	0.573	1.00	38.14	8
	ATOM	647	N	LEU	B	346	-18.071	78.266	1.041	1.00	39.52	7
	ATOM	648	CA	LEU	B	346	-17.563	78.279	2.403	1.00	36.05	6
	ATOM	649	CB	LEU	B	346	-18.311	77.256	3.269	1.00	35.72	6
	ATOM	650	CG	LEU	B	346	-19.800	77.473	3.378	1.00	34.89	6
15	ATOM	651	CD1	LEU	B	346	-20.322	76.678	4.554	1.00	44.09	6
	ATOM	652	CD2	LEU	B	346	-20.086	78.937	3.612	1.00	34.84	6
	ATOM	653	C	LEU	B	346	-16.079	78.018	2.445	1.00	33.52	6
	ATOM	654	O	LEU	B	346	-15.392	78.387	3.394	1.00	35.58	8
	ATOM	655	N	GLY	B	347	-15.586	77.388	1.385	1.00	30.47	7
20	ATOM	656	CA	GLY	B	347	-14.174	77.078	1.305	1.00	33.01	6
	ATOM	657	C	GLY	B	347	-13.768	76.214	2.477	1.00	30.72	6
	ATOM	658	O	GLY	B	347	-14.433	75.243	2.808	1.00	30.89	8
	ATOM	659	N	VAL	B	348	-12.647	76.585	3.087	1.00	31.30	7
	ATOM	660	CA	VAL	B	348	-12.097	75.867	4.227	1.00	31.27	6
25	ATOM	661	CB	VAL	B	348	-10.889	76.609	4.817	1.00	31.66	6
	ATOM	662	CG1	VAL	B	348	-11.292	77.974	5.360	1.00	20.19	6
	ATOM	663	CG2	VAL	B	348	-10.250	75.786	5.905	1.00	24.77	6
	ATOM	664	C	VAL	B	348	-13.136	75.651	5.360	1.00	33.84	6
	ATOM	665	O	VAL	B	348	-13.002	74.707	6.153	1.00	29.99	8
30	ATOM	666	N	VAL	B	349	-14.157	76.518	5.449	1.00	33.31	7
	ATOM	667	CA	VAL	B	349	-15.147	76.339	6.483	1.00	32.23	6
	ATOM	668	CB	VAL	B	349	-16.226	77.393	6.476	1.00	32.59	6
	ATOM	669	CG1	VAL	B	349	-17.342	76.979	7.399	1.00	33.68	6
	ATOM	670	CG2	VAL	B	349	-15.667	78.703	6.959	1.00	32.30	6
35	ATOM	671	C	VAL	B	349	-15.792	74.987	6.380	1.00	34.91	6
	ATOM	672	O	VAL	B	349	-16.055	74.359	7.394	1.00	33.73	8
	ATOM	673	N	SER	B	350	-16.054	74.507	5.176	1.00	32.81	7
	ATOM	674	CA	SER	B	350	-16.695	73.215	5.100	1.00	30.10	6
	ATOM	675	CB	SER	B	350	-16.772	72.697	3.684	1.00	24.95	6
40	ATOM	676	OG	SER	B	350	-17.538	71.502	3.644	1.00	23.16	8
	ATOM	677	C	SER	B	350	-15.910	72.254	5.942	1.00	31.59	6
	ATOM	678	O	SER	B	350	-16.417	71.807	6.950	1.00	37.62	8
	ATOM	679	N	ASP	B	351	-14.675	71.942	5.565	1.00	28.60	7
	ATOM	680	CA	ASP	B	351	-13.905	71.010	6.378	1.00	29.82	6
45	ATOM	681	CB	ASP	B	351	-12.419	71.139	6.050	1.00	27.49	6
	ATOM	682	CG	ASP	B	351	-12.151	71.094	4.585	1.00	30.22	6
	ATOM	683	OD1	ASP	B	351	-12.013	72.174	3.954	1.00	32.61	8
	ATOM	684	OD2	ASP	B	351	-12.064	69.980	4.017	1.00	30.02	8
	ATOM	685	C	ASP	B	351	-14.176	71.343	7.861	1.00	30.63	6
50	ATOM	686	O	ASP	B	351	-14.458	70.474	8.681	1.00	29.54	8
	ATOM	687	N	ALA	B	352	-14.111	72.629	8.177	1.00	25.33	7
	ATOM	688	CA	ALA	B	352	-14.346	73.092	9.533	1.00	28.59	6
	ATOM	689	CB	ALA	B	352	-14.252	74.606	9.572	1.00	20.95	6
	ATOM	690	C	ALA	B	352	-15.690	72.630	10.086	1.00	29.69	6
55	ATOM	691	O	ALA	B	352	-15.757	72.068	11.164	1.00	30.36	8
	ATOM	692	N	ILE	B	353	-16.754	72.884	9.330	1.00	27.63	7
	ATOM	693	CA	ILE	B	353	-18.096	72.506	9.729	1.00	27.55	6
	ATOM	694	CB	ILE	B	353	-19.144	73.129	8.800	1.00	28.04	6

5	ATOM	695	CG2	ILE	B	353	-20.529	72.673	9.195	1.00	23.68	6
	ATOM	696	CG1	ILE	B	353	-19.108	74.657	8.869	1.00	27.33	6
	ATOM	697	CD1	ILE	B	353	-20.141	75.313	7.964	1.00	26.23	6
	ATOM	698	C	ILE	B	353	-18.309	71.002	9.775	1.00	30.88	6
	ATOM	699	O	ILE	B	353	-19.021	70.499	10.639	1.00	31.22	8
10	ATOM	700	N	PHE	B	354	-17.728	70.279	8.822	1.00	29.86	7
	ATOM	701	CA	PHE	B	354	-17.881	68.831	8.797	1.00	31.08	6
	ATOM	702	CB	PHE	B	354	-17.461	68.249	7.439	1.00	28.80	6
	ATOM	703	CG	PHE	B	354	-18.568	68.233	6.405	1.00	28.80	6
	ATOM	704	CD1	PHE	B	354	-19.031	69.403	5.833	1.00	30.96	6
15	ATOM	705	CD2	PHE	B	354	-19.150	67.027	6.034	1.00	29.45	6
	ATOM	706	CE1	PHE	B	354	-20.066	69.362	4.902	1.00	27.12	6
	ATOM	707	CE2	PHE	B	354	-20.186	66.978	5.104	1.00	25.19	6
	ATOM	708	CZ	PHE	B	354	-20.644	68.146	4.535	1.00	28.09	6
	ATOM	709	C	PHE	B	354	-17.041	68.223	9.913	1.00	29.17	6
20	ATOM	710	O	PHE	B	354	-17.544	67.429	10.700	1.00	32.62	8
	ATOM	711	N	ASP	B	355	-15.761	68.593	9.972	1.00	23.86	7
	ATOM	712	CA	ASP	B	355	-14.864	68.090	11.005	1.00	25.34	6
	ATOM	713	CB	ASP	B	355	-13.582	68.929	11.045	1.00	21.41	6
	ATOM	714	CG	ASP	B	355	-12.548	68.456	10.086	1.00	32.08	6
25	ATOM	715	OD1	ASP	B	355	-12.899	68.069	8.944	1.00	33.58	8
	ATOM	716	OD2	ASP	B	355	-11.345	68.477	10.450	1.00	33.20	8
	ATOM	717	C	ASP	B	355	-15.570	68.153	12.357	1.00	27.86	6
	ATOM	718	O	ASP	B	355	-15.430	67.257	13.182	1.00	32.42	8
	ATOM	719	N	LEU	B	356	-16.339	69.223	12.561	1.00	26.84	7
30	ATOM	720	CA	LEU	B	356	-17.085	69.400	13.803	1.00	28.66	6
	ATOM	721	CB	LEU	B	356	-17.832	70.742	13.800	1.00	25.37	6
	ATOM	722	CG	LEU	B	356	-18.655	71.091	15.023	1.00	27.61	6
	ATOM	723	CD1	LEU	B	356	-17.729	71.248	16.191	1.00	25.43	6
	ATOM	724	CD2	LEU	B	356	-19.430	72.363	14.808	1.00	27.49	6
35	ATOM	725	C	LEU	B	356	-18.084	68.260	13.883	1.00	30.44	6
	ATOM	726	O	LEU	B	356	-18.054	67.445	14.804	1.00	31.55	8
	ATOM	727	N	GLY	B	357	-18.972	68.214	12.891	1.00	32.69	7
	ATOM	728	CA	GLY	B	357	-20.001	67.186	12.846	1.00	29.87	6
	ATOM	729	C	GLY	B	357	-19.486	65.832	13.279	1.00	33.12	6
40	ATOM	730	O	GLY	B	357	-20.032	65.246	14.207	1.00	29.41	8
	ATOM	731	N	MET	B	358	-18.444	65.351	12.593	1.00	33.31	7
	ATOM	732	CA	MET	B	358	-17.834	64.066	12.902	1.00	35.87	6
	ATOM	733	CB	MET	B	358	-16.513	63.903	12.151	1.00	34.56	6
	ATOM	734	CG	MET	B	358	-16.649	63.908	10.657	1.00	46.43	6
45	ATOM	735	SD	MET	B	358	-15.094	63.597	9.751	1.00	42.13	16
	ATOM	736	CE	MET	B	358	-14.121	65.063	10.228	1.00	44.29	6
	ATOM	737	C	MET	B	358	-17.552	63.976	14.392	1.00	33.26	6
	ATOM	738	O	MET	B	358	-18.019	63.075	15.075	1.00	36.39	8
	ATOM	739	N	SER	B	359	-16.766	64.933	14.875	1.00	33.31	7
50	ATOM	740	CA	SER	B	359	-16.380	64.998	16.270	1.00	34.39	6
	ATOM	741	CB	SER	B	359	-15.724	66.339	16.541	1.00	30.84	6
	ATOM	742	OG	SER	B	359	-15.130	66.355	17.825	1.00	47.14	8
	ATOM	743	C	SER	B	359	-17.579	64.813	17.169	1.00	36.43	6
	ATOM	744	O	SER	B	359	-17.635	63.853	17.922	1.00	35.46	8
55	ATOM	745	N	LEU	B	360	-18.525	65.744	17.079	1.00	36.74	7
	ATOM	746	CA	LEU	B	360	-19.741	65.729	17.889	1.00	35.44	6
	ATOM	747	CB	LEU	B	360	-20.706	66.817	17.405	1.00	34.16	6
	ATOM	748	CG	LEU	B	360	-20.263	68.255	17.575	1.00	34.59	6

5	ATOM	749	CD1	LEU	B	360	-21.394	69.181	17.212	1.00	33.53	6
	ATOM	750	CD2	LEU	B	360	-19.869	68.486	19.010	1.00	31.69	6
	ATOM	751	C	LEU	B	360	-20.464	64.397	17.924	1.00	38.72	6
	ATOM	752	O	LEU	B	360	-21.021	64.011	18.958	1.00	38.29	8
	ATOM	753	N	SER	B	361	-20.466	63.708	16.791	1.00	40.96	7
10	ATOM	754	CA	SER	B	361	-21.106	62.416	16.721	1.00	45.67	6
	ATOM	755	CB	SER	B	361	-20.532	61.630	15.551	1.00	46.45	6
	ATOM	756	OG	SER	B	361	-20.750	62.314	14.322	1.00	51.81	8
	ATOM	757	C	SER	B	361	-20.895	61.638	18.018	1.00	44.49	6
	ATOM	758	O	SER	B	361	-21.696	60.793	18.362	1.00	46.67	8
15	ATOM	759	N	SER	B	362	-19.811	61.953	18.726	1.00	41.44	7
	ATOM	760	CA	SER	B	362	-19.453	61.309	19.972	1.00	42.13	6
	ATOM	761	CB	SER	B	362	-17.962	61.510	20.234	1.00	42.61	6
	ATOM	762	OG	SER	B	362	-17.164	61.025	19.158	1.00	51.87	8
	ATOM	763	C	SER	B	362	-20.228	61.812	21.174	1.00	38.41	6
20	ATOM	764	O	SER	B	362	-20.602	61.025	22.035	1.00	38.01	8
	ATOM	765	N	PHE	B	363	-20.455	63.123	21.228	1.00	34.55	7
	ATOM	766	CA	PHE	B	363	-21.150	63.735	22.346	1.00	32.96	6
	ATOM	767	CB	PHE	B	363	-21.006	65.245	22.285	1.00	31.99	6
	ATOM	768	CG	PHE	B	363	-19.578	65.719	22.378	1.00	29.97	6
25	ATOM	769	CD1	PHE	B	363	-19.286	67.058	22.447	1.00	30.61	6
	ATOM	770	CD2	PHE	B	363	-18.536	64.800	22.391	1.00	32.02	6
	ATOM	771	CE1	PHE	B	363	-17.966	67.489	22.543	1.00	33.67	6
	ATOM	772	CE2	PHE	B	363	-17.221	65.222	22.484	1.00	30.91	6
	ATOM	773	CZ	PHE	B	363	-16.927	66.557	22.554	1.00	29.33	6
30	ATOM	774	C	PHE	B	363	-22.617	63.361	22.482	1.00	30.52	6
	ATOM	775	O	PHE	B	363	-23.142	63.331	23.596	1.00	32.19	8
	ATOM	776	N	ASN	B	364	-23.279	63.075	21.361	1.00	33.51	7
	ATOM	777	CA	ASN	B	364	-24.683	62.701	21.377	1.00	38.03	6
	ATOM	778	CB	ASN	B	364	-24.855	61.369	22.111	1.00	42.32	6
35	ATOM	779	CG	ASN	B	364	-24.008	60.271	21.524	1.00	53.11	6
	ATOM	780	OD1	ASN	B	364	-24.183	59.895	20.344	1.00	59.51	8
	ATOM	781	ND2	ASN	B	364	-23.102	59.746	22.325	1.00	55.95	7
	ATOM	782	C	ASN	B	364	-25.494	63.771	22.091	1.00	31.89	6
	ATOM	783	O	ASN	B	364	-26.279	63.471	22.990	1.00	30.28	8
40	ATOM	784	N	LEU	B	365	-25.306	65.018	21.673	1.00	27.62	7
	ATOM	785	CA	LEU	B	365	-26.005	66.144	22.280	1.00	29.36	6
	ATOM	786	CB	LEU	B	365	-25.402	67.443	21.743	1.00	27.54	6
	ATOM	787	CG	LEU	B	365	-23.897	67.453	21.738	1.00	38.91	6
	ATOM	788	CD1	LEU	B	365	-23.391	68.766	21.190	1.00	34.47	6
45	ATOM	789	CD2	LEU	B	365	-23.393	67.214	23.143	1.00	34.24	6
	ATOM	790	C	LEU	B	365	-27.496	66.074	21.987	1.00	26.23	6
	ATOM	791	O	LEU	B	365	-27.911	65.790	20.863	1.00	27.06	8
	ATOM	792	N	ASP	B	366	-28.296	66.321	23.022	1.00	25.23	7
	ATOM	793	CA	ASP	B	366	-29.752	66.320	22.878	1.00	26.07	6
50	ATOM	794	CB	ASP	B	366	-30.441	65.651	24.076	1.00	29.68	6
	ATOM	795	CG	ASP	B	366	-30.221	66.374	25.360	1.00	35.74	6
	ATOM	796	OD1	ASP	B	366	-30.277	67.617	25.387	1.00	36.78	8
	ATOM	797	OD2	ASP	B	366	-30.017	65.711	26.410	1.00	41.23	8
	ATOM	798	C	ASP	B	366	-30.230	67.752	22.740	1.00	27.70	6
55	ATOM	799	O	ASP	B	366	-29.552	68.678	23.171	1.00	31.94	8
	ATOM	800	N	ASP	B	367	-31.409	67.913	22.142	1.00	29.18	7
	ATOM	801	CA	ASP	B	367	-32.031	69.225	21.930	1.00	32.72	6
	ATOM	802	CB	ASP	B	367	-33.558	69.106	22.071	1.00	38.04	6

5	ATOM	803	CG	ASP	B	367	-34.172	68.166	21.081	1.00	42.43	6
	ATOM	804	OD1	ASP	B	367	-34.051	68.373	19.854	1.00	35.95	8
	ATOM	805	OD2	ASP	B	367	-34.829	67.188	21.504	1.00	51.42	8
	ATOM	806	C	ASP	B	367	-31.496	70.238	22.959	1.00	33.71	6
	ATOM	807	O	ASP	B	367	-30.791	71.188	22.624	1.00	38.30	8
10	ATOM	808	N	THR	B	368	-31.858	69.997	24.218	1.00	31.06	7
	ATOM	809	CA	THR	B	368	-31.453	70.822	25.344	1.00	26.28	6
	ATOM	810	CB	THR	B	368	-31.567	70.020	26.643	1.00	27.30	6
	ATOM	811	OG1	THR	B	368	-32.916	69.578	26.824	1.00	33.42	8
	ATOM	812	CG2	THR	B	368	-31.143	70.855	27.824	1.00	25.16	6
15	ATOM	813	C	THR	B	368	-30.025	71.315	25.181	1.00	21.13	6
	ATOM	814	O	THR	B	368	-29.746	72.508	25.150	1.00	23.17	8
	ATOM	815	N	GLU	B	369	-29.123	70.354	25.072	1.00	21.32	7
	ATOM	816	CA	GLU	B	369	-27.711	70.634	24.932	1.00	28.00	6
	ATOM	817	CB	GLU	B	369	-26.947	69.306	24.878	1.00	32.79	6
20	ATOM	818	CG	GLU	B	369	-27.229	68.433	26.130	1.00	36.29	6
	ATOM	819	CD	GLU	B	369	-26.689	67.051	26.083	1.00	41.03	6
	ATOM	820	OE1	GLU	B	369	-26.960	66.318	25.102	1.00	42.05	8
	ATOM	821	OE2	GLU	B	369	-25.992	66.645	27.048	1.00	42.03	8
	ATOM	822	C	GLU	B	369	-27.428	71.527	23.731	1.00	25.57	6
25	ATOM	823	O	GLU	B	369	-26.780	72.549	23.886	1.00	20.56	8
	ATOM	824	N	VAL	B	370	-27.922	71.154	22.548	1.00	25.39	7
	ATOM	825	CA	VAL	B	370	-27.710	71.968	21.355	1.00	25.99	6
	ATOM	826	CB	VAL	B	370	-28.457	71.429	20.130	1.00	26.15	6
	ATOM	827	CG1	VAL	B	370	-28.255	72.358	18.953	1.00	27.65	6
30	ATOM	828	CG2	VAL	B	370	-28.014	70.021	19.788	1.00	17.70	6
	ATOM	829	C	VAL	B	370	-28.238	73.346	21.676	1.00	26.49	6
	ATOM	830	O	VAL	B	370	-27.580	74.351	21.445	1.00	28.16	8
	ATOM	831	N	ALA	B	371	-29.450	73.362	22.213	1.00	21.01	7
	ATOM	832	CA	ALA	B	371	-30.145	74.589	22.573	1.00	19.57	6
35	ATOM	833	CB	ALA	B	371	-31.414	74.246	23.335	1.00	18.62	6
	ATOM	834	C	ALA	B	371	-29.256	75.501	23.401	1.00	23.48	6
	ATOM	835	O	ALA	B	371	-28.936	76.613	22.989	1.00	32.67	8
	ATOM	836	N	LEU	B	372	-28.860	75.008	24.571	1.00	22.89	7
	ATOM	837	CA	LEU	B	372	-27.999	75.758	25.472	1.00	23.28	6
40	ATOM	838	CB	LEU	B	372	-27.606	74.860	26.658	1.00	27.76	6
	ATOM	839	CG	LEU	B	372	-28.728	74.524	27.619	1.00	21.18	6
	ATOM	840	CD1	LEU	B	372	-28.272	73.529	28.648	1.00	27.64	6
	ATOM	841	CD2	LEU	B	372	-29.198	75.801	28.284	1.00	20.90	6
	ATOM	842	C	LEU	B	372	-26.769	76.268	24.722	1.00	21.34	6
45	ATOM	843	O	LEU	B	372	-26.439	77.454	24.762	1.00	23.16	8
	ATOM	844	N	LEU	B	373	-26.111	75.349	24.023	1.00	24.42	7
	ATOM	845	CA	LEU	B	373	-24.916	75.669	23.254	1.00	23.78	6
	ATOM	846	CB	LEU	B	373	-24.525	74.446	22.396	1.00	22.18	6
	ATOM	847	CG	LEU	B	373	-23.098	74.283	21.942	1.00	31.52	6
50	ATOM	848	CD1	LEU	B	373	-22.196	74.576	23.100	1.00	31.93	6
	ATOM	849	CD2	LEU	B	373	-22.873	72.889	21.457	1.00	30.24	6
	ATOM	850	C	LEU	B	373	-25.235	76.902	22.405	1.00	25.69	6
	ATOM	851	O	LEU	B	373	-24.491	77.880	22.416	1.00	30.13	8
	ATOM	852	N	GLN	B	374	-26.368	76.842	21.707	1.00	26.24	7
55	ATOM	853	CA	GLN	B	374	-26.836	77.922	20.839	1.00	21.60	6
	ATOM	854	CB	GLN	B	374	-28.196	77.571	20.221	1.00	24.57	6
	ATOM	855	CG	GLN	B	374	-28.188	76.330	19.348	1.00	21.02	6
	ATOM	856	CD	GLN	B	374	-29.538	76.071	18.698	1.00	22.86	6



5	ATOM	857	OE1	GLN	B	374	-29.720	75.049	18.009	1.00	24.07	8
	ATOM	858	NE2	GLN	B	374	-30.473	76.980	18.901	1.00	25.59	7
	ATOM	859	C	GLN	B	374	-26.988	79.249	21.569	1.00	20.66	6
	ATOM	860	O	GLN	B	374	-26.733	80.307	20.994	1.00	24.47	8
	ATOM	861	N	ALA	B	375	-27.429	79.182	22.825	1.00	16.26	7
10	ATOM	862	CA	ALA	B	375	-27.639	80.374	23.631	1.00	17.16	6
	ATOM	863	CB	ALA	B	375	-28.435	80.025	24.865	1.00	19.53	6
	ATOM	864	C	ALA	B	375	-26.304	80.966	24.025	1.00	25.13	6
	ATOM	865	O	ALA	B	375	-26.074	82.154	23.833	1.00	23.81	8
	ATOM	866	N	VAL	B	376	-25.433	80.111	24.568	1.00	24.57	7
15	ATOM	867	CA	VAL	B	376	-24.102	80.526	24.986	1.00	25.80	6
	ATOM	868	CB	VAL	B	376	-23.192	79.321	25.234	1.00	26.48	6
	ATOM	869	CG1	VAL	B	376	-21.806	79.780	25.620	1.00	23.20	6
	ATOM	870	CG2	VAL	B	376	-23.771	78.433	26.310	1.00	19.08	6
	ATOM	871	C	VAL	B	376	-23.510	81.403	23.898	1.00	25.69	6
20	ATOM	872	O	VAL	B	376	-22.796	82.364	24.166	1.00	27.87	8
	ATOM	873	N	LEU	B	377	-23.827	81.049	22.659	1.00	23.09	7
	ATOM	874	CA	LEU	B	377	-23.340	81.774	21.492	1.00	22.86	6
	ATOM	875	CB	LEU	B	377	-23.552	80.920	20.230	1.00	18.50	6
	ATOM	876	CG	LEU	B	377	-22.756	79.638	20.146	1.00	22.65	6
25	ATOM	877	CD1	LEU	B	377	-23.221	78.786	19.000	1.00	16.70	6
	ATOM	878	CD2	LEU	B	377	-21.300	79.995	20.000	1.00	19.58	6
	ATOM	879	C	LEU	B	377	-24.073	83.102	21.384	1.00	26.14	6
	ATOM	880	O	LEU	B	377	-23.464	84.164	21.419	1.00	20.62	8
	ATOM	881	N	LEU	B	378	-25.396	83.023	21.265	1.00	28.99	7
30	ATOM	882	CA	LEU	B	378	-26.228	84.217	21.147	1.00	28.87	6
	ATOM	883	CB	LEU	B	378	-27.696	83.894	21.450	1.00	26.89	6
	ATOM	884	CG	LEU	B	378	-28.648	85.068	21.500	1.00	28.83	6
	ATOM	885	CD1	LEU	B	378	-28.507	85.854	20.225	1.00	27.97	6
	ATOM	886	CD2	LEU	B	378	-30.072	84.605	21.692	1.00	27.69	6
35	ATOM	887	C	LEU	B	378	-25.738	85.280	22.090	1.00	31.09	6
	ATOM	888	O	LEU	B	378	-25.398	86.379	21.651	1.00	31.77	8
	ATOM	889	N	MET	B	379	-25.695	84.931	23.376	1.00	31.44	7
	ATOM	890	CA	MET	B	379	-25.291	85.851	24.434	1.00	32.62	6
	ATOM	891	CB	MET	B	379	-25.797	85.335	25.793	1.00	31.45	6
40	ATOM	892	CG	MET	B	379	-27.332	85.262	25.883	1.00	38.75	6
	ATOM	893	SD	MET	B	379	-28.020	86.915	25.550	1.00	41.27	16
	ATOM	894	CE	MET	B	379	-29.814	86.586	25.513	1.00	35.68	6
	ATOM	895	C	MET	B	379	-23.796	86.129	24.538	1.00	33.72	6
	ATOM	896	O	MET	B	379	-23.246	86.190	25.633	1.00	36.29	8
45	ATOM	897	N	SER	B	380	-23.152	86.335	23.399	1.00	34.49	7
	ATOM	898	CA	SER	B	380	-21.738	86.659	23.391	1.00	33.97	6
	ATOM	899	CB	SER	B	380	-21.132	86.360	22.010	1.00	31.24	6
	ATOM	900	OG	SER	B	380	-21.224	84.978	21.696	1.00	39.42	8
	ATOM	901	C	SER	B	380	-21.635	88.145	23.705	1.00	39.69	6
50	ATOM	902	O	SER	B	380	-22.084	88.989	22.933	1.00	44.64	8
	ATOM	903	N	SER	B	381	-21.053	88.451	24.857	1.00	41.04	7
	ATOM	904	CA	SER	B	381	-20.907	89.826	25.308	1.00	44.91	6
	ATOM	905	CB	SER	B	381	-20.610	89.832	26.797	1.00	44.50	6
	ATOM	906	OG	SER	B	381	-19.351	89.229	27.037	1.00	45.42	8
55	ATOM	907	C	SER	B	381	-19.815	90.614	24.602	1.00	44.59	6
	ATOM	908	O	SER	B	381	-19.725	91.825	24.751	1.00	49.32	8
	ATOM	909	N	ASP	B	382	-18.977	89.922	23.848	1.00	43.75	7
	ATOM	910	CA	ASP	B	382	-17.886	90.556	23.144	1.00	43.93	6

5	ATOM	911	CB	ASP	B	382	-16.727	89.562	23.028	1.00	48.39	6
	ATOM	912	CG	ASP	B	382	-17.142	88.232	22.471	1.00	53.23	6
	ATOM	913	OD1	ASP	B	382	-18.102	87.621	23.002	1.00	56.97	8
	ATOM	914	OD2	ASP	B	382	-16.513	87.753	21.480	1.00	58.91	8
	ATOM	915	C	ASP	B	382	-18.191	91.172	21.772	1.00	41.09	6
10	ATOM	916	O	ASP	B	382	-17.366	91.899	21.229	1.00	40.93	8
	ATOM	917	N	ARG	B	383	-19.369	90.908	21.224	1.00	42.63	7
	ATOM	918	CA	ARG	B	383	-19.698	91.445	19.934	1.00	43.32	6
	ATOM	919	CB	ARG	B	383	-21.131	91.101	19.557	1.00	42.31	6
	ATOM	920	CG	ARG	B	383	-21.619	89.672	19.811	1.00	40.83	6
15	ATOM	921	CD	ARG	B	383	-21.144	88.627	18.804	1.00	38.09	6
	ATOM	922	NE	ARG	B	383	-21.922	87.415	18.943	1.00	37.33	7
	ATOM	923	CZ	ARG	B	383	-21.584	86.250	18.411	1.00	38.35	6
	ATOM	924	NH1	ARG	B	383	-20.465	86.143	17.700	1.00	33.70	7
	ATOM	925	NH2	ARG	B	383	-22.369	85.196	18.604	1.00	35.46	7
20	ATOM	926	C	ARG	B	383	-19.591	92.958	20.007	1.00	44.96	6
	ATOM	927	O	ARG	B	383	-20.050	93.577	20.980	1.00	45.60	8
	ATOM	928	N	PRO	B	384	-18.975	93.579	19.005	1.00	45.33	7
	ATOM	929	CD	PRO	B	384	-18.395	92.881	17.854	1.00	46.85	6
	ATOM	930	CA	PRO	B	384	-18.808	95.035	18.947	1.00	47.37	6
25	ATOM	931	CB	PRO	B	384	-17.868	95.255	17.764	1.00	46.90	6
	ATOM	932	CG	PRO	B	384	-17.575	93.934	17.187	1.00	46.41	6
	ATOM	933	C	PRO	B	384	-20.125	95.778	18.762	1.00	48.29	6
	ATOM	934	O	PRO	B	384	-21.048	95.277	18.120	1.00	48.34	8
	ATOM	935	N	GLY	B	385	-20.185	96.994	19.314	1.00	49.88	7
30	ATOM	936	CA	GLY	B	385	-21.371	97.838	19.192	1.00	50.35	6
	ATOM	937	C	GLY	B	385	-22.410	97.615	20.265	1.00	50.70	6
	ATOM	938	O	GLY	B	385	-23.382	98.363	20.374	1.00	53.48	8
	ATOM	939	N	LEU	B	386	-22.205	96.557	21.044	1.00	49.04	7
	ATOM	940	CA	LEU	B	386	-23.136	96.211	22.101	1.00	50.53	6
35	ATOM	941	CB	LEU	B	386	-22.640	94.972	22.853	1.00	45.17	6
	ATOM	942	CG	LEU	B	386	-22.744	93.653	22.121	1.00	48.26	6
	ATOM	943	CD1	LEU	B	386	-22.122	92.525	22.938	1.00	41.68	6
	ATOM	944	CD2	LEU	B	386	-24.215	93.376	21.852	1.00	38.40	6
	ATOM	945	C	LEU	B	386	-23.322	97.357	23.058	1.00	52.13	6
40	ATOM	946	O	LEU	B	386	-22.438	98.182	23.234	1.00	53.67	8
	ATOM	947	N	ALA	B	387	-24.499	97.398	23.666	1.00	53.42	7
	ATOM	948	CA	ALA	B	387	-24.830	98.441	24.624	1.00	56.01	6
	ATOM	949	CB	ALA	B	387	-26.223	98.993	24.339	1.00	56.47	6
	ATOM	950	C	ALA	B	387	-24.775	97.853	26.024	1.00	55.52	6
45	ATOM	951	O	ALA	B	387	-23.798	98.027	26.753	1.00	53.75	8
	ATOM	952	N	CYS	B	388	-25.843	97.145	26.371	1.00	56.03	7
	ATOM	953	CA	CYS	B	388	-26.000	96.525	27.673	1.00	59.57	6
	ATOM	954	CB	CYS	B	388	-27.469	96.134	27.839	1.00	59.23	6
	ATOM	955	SG	CYS	B	388	-28.620	97.392	27.264	1.00	58.64	16
50	ATOM	956	C	CYS	B	388	-25.105	95.283	27.798	1.00	62.18	6
	ATOM	957	O	CYS	B	388	-25.590	94.164	27.868	1.00	67.88	8
	ATOM	958	N	VAL	B	389	-23.789	95.510	27.824	1.00	60.78	7
	ATOM	959	CA	VAL	B	389	-22.797	94.434	27.959	1.00	57.70	6
	ATOM	960	CB	VAL	B	389	-21.355	94.976	27.998	1.00	57.09	6
55	ATOM	961	CG1	VAL	B	389	-20.361	93.832	28.085	1.00	59.03	6
	ATOM	962	CG2	VAL	B	389	-21.065	95.845	26.791	1.00	53.98	6
	ATOM	963	C	VAL	B	389	-23.078	93.642	29.230	1.00	57.77	6
	ATOM	964	O	VAL	B	389	-23.727	92.602	29.203	1.00	60.94	8

5	ATOM	965	N	ALA	B	390	-22.561	94.159	30.332	1.00	52.68	7
	ATOM	966	CA	ALA	B	390	-22.684	93.570	31.659	1.00	48.41	6
	ATOM	967	CB	ALA	B	390	-22.650	94.681	32.716	1.00	45.19	6
	ATOM	968	C	ALA	B	390	-23.905	92.697	31.877	1.00	47.63	6
	ATOM	969	O	ALA	B	390	-23.784	91.576	32.369	1.00	51.95	8
10	ATOM	970	N	ARG	B	391	-25.075	93.216	31.498	1.00	47.11	7
	ATOM	971	CA	ARG	B	391	-26.330	92.481	31.656	1.00	51.64	6
	ATOM	972	CB	ARG	B	391	-27.502	93.318	31.122	1.00	54.22	6
	ATOM	973	CG	ARG	B	391	-28.887	92.713	31.430	1.00	64.20	6
	ATOM	974	CD	ARG	B	391	-30.059	93.582	30.929	1.00	73.80	6
15	ATOM	975	NE	ARG	B	391	-31.361	93.097	31.378	1.00	79.76	7
	ATOM	976	CZ	ARG	B	391	-31.736	93.015	32.656	1.00	84.27	6
	ATOM	977	NH1	ARG	B	391	-30.887	93.372	33.625	1.00	85.28	7
	ATOM	978	NH2	ARG	B	391	-32.957	92.566	32.955	1.00	86.84	7
	ATOM	979	C	ARG	B	391	-26.277	91.133	30.940	1.00	48.18	6
20	ATOM	980	O	ARG	B	391	-26.724	90.119	31.465	1.00	49.57	8
	ATOM	981	N	ILE	B	392	-25.743	91.167	29.718	1.00	45.01	7
	ATOM	982	CA	ILE	B	392	-25.592	89.999	28.867	1.00	48.77	6
	ATOM	983	CB	ILE	B	392	-25.112	90.424	27.469	1.00	46.45	6
	ATOM	984	CG2	ILE	B	392	-24.805	89.221	26.614	1.00	42.35	6
25	ATOM	985	CG1	ILE	B	392	-26.178	91.283	26.768	1.00	49.69	6
	ATOM	986	CD1	ILE	B	392	-25.762	91.768	25.386	1.00	51.09	6
	ATOM	987	C	ILE	B	392	-24.671	88.935	29.462	1.00	50.90	6
	ATOM	988	O	ILE	B	392	-25.086	87.780	29.605	1.00	52.21	8
	ATOM	989	N	GLU	B	393	-23.431	89.298	29.790	1.00	50.43	7
30	ATOM	990	CA	GLU	B	393	-22.504	88.328	30.378	1.00	50.30	6
	ATOM	991	CB	GLU	B	393	-21.314	89.022	31.044	1.00	53.97	6
	ATOM	992	CG	GLU	B	393	-20.063	89.005	30.209	1.00	62.18	6
	ATOM	993	CD	GLU	B	393	-18.877	89.415	30.976	1.00	67.69	6
	ATOM	994	OE1	GLU	B	393	-17.709	89.264	30.656	1.00	66.42	8
35	ATOM	995	OE2	GLU	B	393	-18.897	89.976	32.052	1.00	70.64	8
	ATOM	996	C	GLU	B	393	-23.251	87.477	31.416	1.00	49.31	6
	ATOM	997	O	GLU	B	393	-23.226	86.260	31.303	1.00	49.53	8
	ATOM	998	N	LYS	B	394	-23.898	88.153	32.409	1.00	46.07	7
	ATOM	999	CA	LYS	B	394	-24.721	87.579	33.506	1.00	45.76	6
40	ATOM	1000	CB	LYS	B	394	-25.594	88.693	34.161	1.00	43.85	6
	ATOM	1001	C	LYS	B	394	-25.626	86.548	32.851	1.00	46.69	6
	ATOM	1002	O	LYS	B	394	-25.772	85.430	33.329	1.00	49.13	8
	ATOM	1003	N	TYR	B	395	-26.203	86.948	31.719	1.00	46.57	7
	ATOM	1004	CA	TYR	B	395	-27.076	86.078	30.938	1.00	43.33	6
45	ATOM	1005	CB	TYR	B	395	-27.621	86.821	29.716	1.00	48.44	6
	ATOM	1006	CG	TYR	B	395	-28.827	87.688	29.980	1.00	53.83	6
	ATOM	1007	CD1	TYR	B	395	-29.204	88.680	29.080	1.00	56.43	6
	ATOM	1008	CE1	TYR	B	395	-30.331	89.469	29.309	1.00	59.73	6
	ATOM	1009	CD2	TYR	B	395	-29.596	87.509	31.113	1.00	56.47	6
50	ATOM	1010	CE2	TYR	B	395	-30.723	88.295	31.346	1.00	62.60	6
	ATOM	1011	CZ	TYR	B	395	-31.090	89.281	30.446	1.00	63.18	6
	ATOM	1012	OH	TYR	B	395	-32.189	90.068	30.671	1.00	64.46	8
	ATOM	1013	C	TYR	B	395	-26.276	84.867	30.485	1.00	37.30	6
	ATOM	1014	O	TYR	B	395	-26.611	83.737	30.825	1.00	34.10	8
55	ATOM	1015	N	GLN	B	396	-25.213	85.108	29.718	1.00	31.92	7
	ATOM	1016	CA	GLN	B	396	-24.380	84.018	29.244	1.00	34.81	6
	ATOM	1017	CB	GLN	B	396	-23.176	84.550	28.464	1.00	32.64	6
	ATOM	1018	CG	GLN	B	396	-22.184	83.470	28.103	1.00	29.57	6

5	ATOM	1019	CD	GLN	B	396	-21.214	83.871	27.016	1.00	29.46	6
	ATOM	1020	OE1	GLN	B	396	-20.547	84.930	27.109	1.00	34.65	8
	ATOM	1021	NE2	GLN	B	396	-21.112	83.032	25.992	1.00	27.21	7
	ATOM	1022	C	GLN	B	396	-23.908	83.207	30.434	1.00	37.13	6
	ATOM	1023	O	GLN	B	396	-23.876	81.986	30.384	1.00	37.36	8
10	ATOM	1024	N	ASP	B	397	-23.544	83.903	31.508	1.00	38.61	7
	ATOM	1025	CA	ASP	B	397	-23.069	83.250	32.717	1.00	40.37	6
	ATOM	1026	CB	ASP	B	397	-22.617	84.297	33.754	1.00	40.51	6
	ATOM	1027	CG	ASP	B	397	-21.360	85.025	33.352	1.00	43.77	6
	ATOM	1028	OD1	ASP	B	397	-20.337	84.366	33.054	1.00	46.50	8
15	ATOM	1029	OD2	ASP	B	397	-21.343	86.287	33.350	1.00	51.34	8
	ATOM	1030	C	ASP	B	397	-24.223	82.422	33.267	1.00	38.62	6
	ATOM	1031	O	ASP	B	397	-24.023	81.327	33.778	1.00	39.20	8
	ATOM	1032	N	SER	B	398	-25.432	82.962	33.138	1.00	37.84	7
	ATOM	1033	CA	SER	B	398	-26.633	82.293	33.622	1.00	37.80	6
20	ATOM	1034	CB	SER	B	398	-27.830	83.246	33.501	1.00	34.28	6
	ATOM	1035	OG	SER	B	398	-28.995	82.715	34.114	1.00	46.60	8
	ATOM	1036	C	SER	B	398	-26.911	80.997	32.867	1.00	38.41	6
	ATOM	1037	O	SER	B	398	-27.454	80.047	33.433	1.00	39.98	8
	ATOM	1038	N	PHE	B	399	-26.546	80.963	31.587	1.00	34.82	7
25	ATOM	1039	CA	PHE	B	399	-26.772	79.768	30.781	1.00	35.96	6
	ATOM	1040	CB	PHE	B	399	-26.892	80.100	29.293	1.00	35.75	6
	ATOM	1041	CG	PHE	B	399	-28.211	80.717	28.906	1.00	39.30	6
	ATOM	1042	CD1	PHE	B	399	-28.466	82.056	29.109	1.00	39.86	6
	ATOM	1043	CD2	PHE	B	399	-29.194	79.938	28.355	1.00	36.81	6
30	ATOM	1044	CE1	PHE	B	399	-29.700	82.602	28.739	1.00	41.25	6
	ATOM	1045	CE2	PHE	B	399	-30.424	80.483	27.987	1.00	43.61	6
	ATOM	1046	CZ	PHE	B	399	-30.677	81.813	28.181	1.00	40.34	6
	ATOM	1047	C	PHE	B	399	-25.658	78.754	30.976	1.00	33.48	6
	ATOM	1048	O	PHE	B	399	-25.927	77.589	31.256	1.00	26.86	8
35	ATOM	1049	N	LEU	B	400	-24.408	79.187	30.796	1.00	31.47	7
	ATOM	1050	CA	LEU	B	400	-23.275	78.291	30.945	1.00	37.41	6
	ATOM	1051	CB	LEU	B	400	-21.976	79.091	31.030	1.00	34.24	6
	ATOM	1052	CG	LEU	B	400	-21.470	79.642	29.726	1.00	35.10	6
	ATOM	1053	CD1	LEU	B	400	-20.121	80.304	29.917	1.00	26.60	6
40	ATOM	1054	CD2	LEU	B	400	-21.326	78.488	28.759	1.00	29.44	6
	ATOM	1055	C	LEU	B	400	-23.430	77.376	32.145	1.00	38.84	6
	ATOM	1056	O	LEU	B	400	-23.366	76.157	32.007	1.00	40.38	8
	ATOM	1057	N	LEU	B	401	-23.639	77.968	33.321	1.00	42.79	7
	ATOM	1058	CA	LEU	B	401	-23.801	77.181	34.537	1.00	43.48	6
45	ATOM	1059	CB	LEU	B	401	-24.226	78.067	35.712	1.00	44.73	6
	ATOM	1060	CG	LEU	B	401	-24.378	77.303	37.012	1.00	51.39	6
	ATOM	1061	CD1	LEU	B	401	-22.990	76.844	37.484	1.00	50.11	6
	ATOM	1062	CD2	LEU	B	401	-25.027	78.163	38.083	1.00	49.30	6
	ATOM	1063	C	LEU	B	401	-24.854	76.095	34.311	1.00	41.62	6
50	ATOM	1064	O	LEU	B	401	-24.576	74.900	34.427	1.00	45.14	8
	ATOM	1065	N	ALA	B	402	-26.068	76.532	33.997	1.00	37.92	7
	ATOM	1066	CA	ALA	B	402	-27.177	75.631	33.752	1.00	29.90	6
	ATOM	1067	CB	ALA	B	402	-28.361	76.433	33.200	1.00	30.70	6
	ATOM	1068	C	ALA	B	402	-26.779	74.521	32.773	1.00	28.88	6
55	ATOM	1069	O	ALA	B	402	-27.078	73.347	32.996	1.00	32.14	8
	ATOM	1070	N	PHE	B	403	-26.091	74.908	31.698	1.00	31.07	7
	ATOM	1071	CA	PHE	B	403	-25.655	73.970	30.673	1.00	29.90	6
	ATOM	1072	CB	PHE	B	403	-24.847	74.715	29.607	1.00	27.03	6

5	ATOM	1073	CG	PHE B 403	-24.557	73.908	28.359	1.00	26.97	6
	ATOM	1074	CD1	PHE B 403	-23.916	74.494	27.272	1.00	25.55	6
	ATOM	1075	CD2	PHE B 403	-24.939	72.583	28.271	1.00	19.75	6
	ATOM	1076	CE1	PHE B 403	-23.670	73.765	26.104	1.00	27.90	6
	ATOM	1077	CE2	PHE B 403	-24.693	71.848	27.102	1.00	22.56	6
10	ATOM	1078	CZ	PHE B 403	-24.057	72.439	26.020	1.00	22.24	6
	ATOM	1079	C	PHE B 403	-24.810	72.902	31.329	1.00	28.82	6
	ATOM	1080	O	PHE B 403	-25.092	71.726	31.205	1.00	26.00	8
	ATOM	1081	N	GLU B 404	-23.776	73.335	32.037	1.00	30.25	7
	ATOM	1082	CA	GLU B 404	-22.865	72.419	32.712	1.00	34.03	6
15	ATOM	1083	CB	GLU B 404	-21.835	73.215	33.527	1.00	39.45	6
	ATOM	1084	CG	GLU B 404	-20.654	72.384	34.068	1.00	47.68	6
	ATOM	1085	CD	GLU B 404	-19.750	73.129	34.996	1.00	54.02	6
	ATOM	1086	OE1	GLU B 404	-19.372	74.290	34.701	1.00	57.27	8
	ATOM	1087	OE2	GLU B 404	-19.369	72.555	36.048	1.00	63.85	8
20	ATOM	1088	C	GLU B 404	-23.645	71.509	33.642	1.00	36.01	6
	ATOM	1089	O	GLU B 404	-23.470	70.292	33.640	1.00	38.64	8
	ATOM	1090	N	HIS B 405	-24.492	72.131	34.458	1.00	29.56	7
	ATOM	1091	CA	HIS B 405	-25.306	71.387	35.405	1.00	31.69	6
	ATOM	1092	CB	HIS B 405	-26.245	72.324	36.173	1.00	33.75	6
25	ATOM	1093	CG	HIS B 405	-25.536	73.185	37.163	1.00	34.75	6
	ATOM	1094	CD2	HIS B 405	-24.234	73.286	37.524	1.00	34.58	6
	ATOM	1095	ND1	HIS B 405	-26.223	74.101	37.969	1.00	32.43	7
	ATOM	1096	CE1	HIS B 405	-25.334	74.703	38.769	1.00	36.15	6
	ATOM	1097	NE2	HIS B 405	-24.139	74.222	38.511	1.00	39.84	7
30	ATOM	1098	C	HIS B 405	-26.106	70.342	34.648	1.00	34.21	6
	ATOM	1099	O	HIS B 405	-26.087	69.160	35.006	1.00	37.06	8
	ATOM	1100	N	TYR B 406	-26.806	70.776	33.598	1.00	30.83	7
	ATOM	1101	CA	TYR B 406	-27.592	69.853	32.796	1.00	28.85	6
	ATOM	1102	CB	TYR B 406	-28.192	70.537	31.579	1.00	31.48	6
35	ATOM	1103	CG	TYR B 406	-28.991	69.576	30.730	1.00	23.49	6
	ATOM	1104	CD1	TYR B 406	-30.179	69.047	31.196	1.00	19.42	6
	ATOM	1105	CE1	TYR B 406	-30.893	68.128	30.441	1.00	23.80	6
	ATOM	1106	CD2	TYR B 406	-28.525	69.152	29.496	1.00	21.81	6
	ATOM	1107	CE2	TYR B 406	-29.241	68.228	28.740	1.00	24.64	6
40	ATOM	1108	CZ	TYR B 406	-30.420	67.713	29.217	1.00	21.56	6
	ATOM	1109	OH	TYR B 406	-31.120	66.802	28.480	1.00	24.96	8
	ATOM	1110	C	TYR B 406	-26.697	68.725	32.304	1.00	24.24	6
	ATOM	1111	O	TYR B 406	-27.155	67.609	32.110	1.00	27.08	8
	ATOM	1112	N	ILE B 407	-25.422	69.056	32.084	1.00	25.76	7
45	ATOM	1113	CA	ILE B 407	-24.428	68.092	31.628	1.00	33.75	6
	ATOM	1114	CB	ILE B 407	-23.090	68.778	31.274	1.00	34.23	6
	ATOM	1115	CG2	ILE B 407	-21.959	67.774	31.230	1.00	32.46	6
	ATOM	1116	CG1	ILE B 407	-23.214	69.514	29.936	1.00	43.30	6
	ATOM	1117	CD1	ILE B 407	-23.655	68.612	28.804	1.00	40.40	6
50	ATOM	1118	C	ILE B 407	-24.191	67.004	32.658	1.00	39.03	6
	ATOM	1119	O	ILE B 407	-24.178	65.806	32.343	1.00	35.18	8
	ATOM	1120	N	ASN B 408	-23.990	67.425	33.894	1.00	37.25	7
	ATOM	1121	CA	ASN B 408	-23.739	66.475	34.943	1.00	37.01	6
	ATOM	1122	CB	ASN B 408	-23.524	67.221	36.256	1.00	32.27	6
55	ATOM	1123	CG	ASN B 408	-22.296	68.137	36.202	1.00	33.56	6
	ATOM	1124	OD1	ASN B 408	-21.194	67.696	35.823	1.00	31.99	8
	ATOM	1125	ND2	ASN B 408	-22.478	69.397	36.604	1.00	31.23	7
	ATOM	1126	C	ASN B 408	-24.876	65.453	35.036	1.00	38.14	6

5	ATOM	1127	O	ASN	B	408	-24.624	64.253	35.105	1.00	42.16	8
	ATOM	1128	N	TYR	B	409	-26.122	65.924	35.003	1.00	35.62	7
	ATOM	1129	CA	TYR	B	409	-27.273	65.024	35.073	1.00	35.91	6
	ATOM	1130	CB	TYR	B	409	-28.597	65.787	34.931	1.00	34.41	6
	ATOM	1131	CG	TYR	B	409	-29.788	64.868	34.685	1.00	38.73	6
10	ATOM	1132	CD1	TYR	B	409	-30.064	63.819	35.549	1.00	41.34	6
	ATOM	1133	CE1	TYR	B	409	-31.130	62.962	35.309	1.00	47.16	6
	ATOM	1134	CD2	TYR	B	409	-30.613	65.037	33.579	1.00	46.20	6
	ATOM	1135	CE2	TYR	B	409	-31.684	64.176	33.341	1.00	50.74	6
	ATOM	1136	CZ	TYR	B	409	-31.942	63.143	34.206	1.00	50.88	6
15	ATOM	1137	OH	TYR	B	409	-33.002	62.312	33.978	1.00	53.14	8
	ATOM	1138	C	TYR	B	409	-27.215	64.020	33.951	1.00	38.16	6
	ATOM	1139	O	TYR	B	409	-27.558	62.857	34.111	1.00	41.83	8
	ATOM	1140	N	ARG	B	410	-26.824	64.528	32.796	1.00	42.25	7
	ATOM	1141	CA	ARG	B	410	-26.734	63.739	31.594	1.00	42.83	6
20	ATOM	1142	CB	ARG	B	410	-26.350	64.646	30.441	1.00	36.83	6
	ATOM	1143	CG	ARG	B	410	-27.440	65.585	29.945	1.00	34.32	6
	ATOM	1144	CD	ARG	B	410	-28.284	64.863	28.917	1.00	36.62	6
	ATOM	1145	NE	ARG	B	410	-27.455	64.378	27.829	1.00	38.64	7
	ATOM	1146	CZ	ARG	B	410	-27.926	63.656	26.824	1.00	35.73	6
25	ATOM	1147	NH1	ARG	B	410	-29.234	63.379	26.782	1.00	33.17	7
	ATOM	1148	NH2	ARG	B	410	-27.095	63.227	25.868	1.00	32.70	7
	ATOM	1149	C	ARG	B	410	-25.688	62.664	31.733	1.00	46.67	6
	ATOM	1150	O	ARG	B	410	-25.859	61.547	31.257	1.00	41.78	8
	ATOM	1151	N	LYS	B	411	-24.602	63.028	32.413	1.00	52.99	7
30	ATOM	1152	CA	LYS	B	411	-23.471	62.145	32.609	1.00	58.32	6
	ATOM	1153	CB	LYS	B	411	-23.684	61.249	33.833	1.00	64.99	6
	ATOM	1154	CG	LYS	B	411	-24.998	60.544	33.968	1.00	70.48	6
	ATOM	1155	CD	LYS	B	411	-25.070	59.887	35.349	1.00	77.18	6
	ATOM	1156	CE	LYS	B	411	-26.272	58.944	35.474	1.00	84.30	6
35	ATOM	1157	NZ	LYS	B	411	-26.286	58.242	36.809	1.00	86.48	7
	ATOM	1158	C	LYS	B	411	-23.172	61.341	31.365	1.00	56.66	6
	ATOM	1159	O	LYS	B	411	-23.574	60.199	31.210	1.00	55.47	8
	ATOM	1160	N	HIS	B	412	-22.458	62.026	30.479	1.00	54.67	7
	ATOM	1161	CA	HIS	B	412	-22.019	61.474	29.214	1.00	48.67	6
40	ATOM	1162	CB	HIS	B	412	-21.500	62.599	28.310	1.00	43.14	6
	ATOM	1163	CG	HIS	B	412	-22.559	63.501	27.784	1.00	41.36	6
	ATOM	1164	CD2	HIS	B	412	-23.159	64.603	28.299	1.00	35.44	6
	ATOM	1165	ND1	HIS	B	412	-23.163	63.290	26.539	1.00	38.19	7
	ATOM	1166	CE1	HIS	B	412	-24.076	64.238	26.353	1.00	34.75	6
45	ATOM	1167	NE2	HIS	B	412	-24.090	65.034	27.396	1.00	35.52	7
	ATOM	1168	C	HIS	B	412	-20.894	60.596	29.644	1.00	46.35	6
	ATOM	1169	O	HIS	B	412	-20.218	60.892	30.644	1.00	42.73	8
	ATOM	1170	N	HIS	B	413	-20.708	59.469	28.973	1.00	48.92	7
	ATOM	1171	CA	HIS	B	413	-19.593	58.614	29.371	1.00	53.15	6
50	ATOM	1172	CB	HIS	B	413	-20.022	57.147	29.421	1.00	55.27	6
	ATOM	1173	CG	HIS	B	413	-20.814	56.823	30.636	1.00	58.77	6
	ATOM	1174	CD2	HIS	B	413	-22.019	56.223	30.822	1.00	61.65	6
	ATOM	1175	ND1	HIS	B	413	-20.360	57.159	31.921	1.00	60.31	7
	ATOM	1176	CE1	HIS	B	413	-21.267	56.758	32.809	1.00	63.01	6
55	ATOM	1177	NE2	HIS	B	413	-22.270	56.193	32.171	1.00	62.93	7
	ATOM	1178	C	HIS	B	413	-18.426	58.862	28.438	1.00	53.19	6
	ATOM	1179	O	HIS	B	413	-17.975	57.996	27.699	1.00	54.93	8
	ATOM	1180	N	VAL	B	414	-17.970	60.113	28.521	1.00	53.77	7

5	ATOM	1181	CA	VAL B 414	-16.845	60.674	27.788	1.00	51.06	6
	ATOM	1182	CB	VAL B 414	-17.317	61.498	26.586	1.00	51.49	6
	ATOM	1183	CG1	VAL B 414	-16.133	62.122	25.891	1.00	45.22	6
	ATOM	1184	CG2	VAL B 414	-18.095	60.631	25.617	1.00	52.67	6
	ATOM	1185	C	VAL B 414	-16.096	61.557	28.775	1.00	54.28	6
10	ATOM	1186	O	VAL B 414	-16.700	62.283	29.574	1.00	55.49	8
	ATOM	1187	N	THR B 415	-14.770	61.466	28.742	1.00	56.28	7
	ATOM	1188	CA	THR B 415	-13.919	62.234	29.669	1.00	57.83	6
	ATOM	1189	CB	THR B 415	-12.488	61.686	29.658	1.00	59.64	6
	ATOM	1190	OG1	THR B 415	-11.618	62.572	30.373	1.00	66.69	8
15	ATOM	1191	CG2	THR B 415	-11.988	61.483	28.227	1.00	59.42	6
	ATOM	1192	C	THR B 415	-13.840	63.726	29.352	1.00	56.98	6
	ATOM	1193	O	THR B 415	-13.987	64.135	28.216	1.00	55.70	8
	ATOM	1194	N	HIS B 416	-13.598	64.522	30.387	1.00	57.44	7
	ATOM	1195	CA	HIS B 416	-13.485	65.972	30.237	1.00	57.34	6
20	ATOM	1196	CB	HIS B 416	-12.114	66.326	29.653	1.00	61.35	6
	ATOM	1197	CG	HIS B 416	-10.968	65.931	30.513	1.00	69.78	6
	ATOM	1198	CD2	HIS B 416	-9.930	65.082	30.307	1.00	71.42	6
	ATOM	1199	ND1	HIS B 416	-10.756	66.480	31.787	1.00	72.49	7
	ATOM	1200	CE1	HIS B 416	-9.631	65.973	32.281	1.00	75.50	6
25	ATOM	1201	NE2	HIS B 416	-9.120	65.131	31.408	1.00	73.91	7
	ATOM	1202	C	HIS B 416	-14.560	66.515	29.320	1.00	53.79	6
	ATOM	1203	O	HIS B 416	-14.334	67.477	28.591	1.00	52.81	8
	ATOM	1204	N	PHE B 417	-15.746	65.921	29.372	1.00	48.05	7
	ATOM	1205	CA	PHE B 417	-16.841	66.329	28.505	1.00	47.99	6
30	ATOM	1206	CB	PHE B 417	-18.152	65.694	28.937	1.00	46.11	6
	ATOM	1207	CG	PHE B 417	-19.233	65.781	27.898	1.00	44.27	6
	ATOM	1208	CD1	PHE B 417	-19.280	64.856	26.870	1.00	41.79	6
	ATOM	1209	CD2	PHE B 417	-20.118	66.846	27.893	1.00	40.23	6
	ATOM	1210	CE1	PHE B 417	-20.233	64.959	25.869	1.00	44.30	6
35	ATOM	1211	CE2	PHE B 417	-21.072	66.955	26.893	1.00	36.80	6
	ATOM	1212	CZ	PHE B 417	-21.119	66.016	25.866	1.00	40.69	6
	ATOM	1213	C	PHE B 417	-17.020	67.833	28.423	1.00	46.69	6
	ATOM	1214	O	PHE B 417	-16.799	68.423	27.380	1.00	43.35	8
	ATOM	1215	N	TRP B 418	-17.448	68.452	29.516	1.00	45.14	7
40	ATOM	1216	CA	TRP B 418	-17.681	69.889	29.508	1.00	44.89	6
	ATOM	1217	CB	TRP B 418	-18.045	70.398	30.898	1.00	42.24	6
	ATOM	1218	CG	TRP B 418	-18.162	71.905	31.018	1.00	47.11	6
	ATOM	1219	CD2	TRP B 418	-19.298	72.699	30.620	1.00	46.98	6
	ATOM	1220	CE2	TRP B 418	-18.953	74.061	30.850	1.00	48.94	6
45	ATOM	1221	CE3	TRP B 418	-20.560	72.401	30.086	1.00	45.23	6
	ATOM	1222	CD1	TRP B 418	-17.223	72.778	31.462	1.00	46.24	6
	ATOM	1223	NE1	TRP B 418	-17.690	74.071	31.368	1.00	50.63	7
	ATOM	1224	CZ2	TRP B 418	-19.819	75.109	30.571	1.00	45.46	6
	ATOM	1225	CZ3	TRP B 418	-21.422	73.447	29.809	1.00	44.50	6
50	ATOM	1226	CH2	TRP B 418	-21.065	74.777	30.039	1.00	47.55	6
	ATOM	1227	C	TRP B 418	-16.502	70.662	28.956	1.00	43.88	6
	ATOM	1228	O	TRP B 418	-16.671	71.424	27.986	1.00	43.17	8
	ATOM	1229	N	PRO B 419	-15.292	70.490	29.519	1.00	43.55	7
	ATOM	1230	CD	PRO B 419	-14.967	69.551	30.599	1.00	41.52	6
55	ATOM	1231	CA	PRO B 419	-14.120	71.223	29.011	1.00	41.48	6
	ATOM	1232	CB	PRO B 419	-12.956	70.582	29.724	1.00	39.21	6
	ATOM	1233	CG	PRO B 419	-13.521	69.703	30.774	1.00	39.25	6
	ATOM	1234	C	PRO B 419	-14.035	71.067	27.479	1.00	36.28	6

5	ATOM	1235	O	PRO B 419	-13.690	72.001	26.754	1.00	37.08	8
	ATOM	1236	N	LYS B 420	-14.330	69.871	26.976	1.00	35.96	7
	ATOM	1237	CA	LYS B 420	-14.278	69.609	25.538	1.00	40.82	6
	ATOM	1238	CB	LYS B 420	-14.452	68.103	25.271	1.00	40.78	6
	ATOM	1239	CG	LYS B 420	-13.349	67.214	25.830	1.00	48.62	6
10	ATOM	1240	CD	LYS B 420	-13.565	65.746	25.480	1.00	55.12	6
	ATOM	1241	CE	LYS B 420	-12.427	64.892	26.017	1.00	53.26	6
	ATOM	1242	NZ	LYS B 420	-12.582	63.457	25.608	1.00	52.69	7
	ATOM	1243	C	LYS B 420	-15.414	70.374	24.875	1.00	40.29	6
	ATOM	1244	O	LYS B 420	-15.225	71.015	23.851	1.00	39.66	8
15	ATOM	1245	N	LEU B 421	-16.591	70.300	25.499	1.00	38.33	7
	ATOM	1246	CA	LEU B 421	-17.796	70.958	25.001	1.00	37.60	6
	ATOM	1247	CB	LEU B 421	-18.970	70.702	25.965	1.00	43.66	6
	ATOM	1248	CG	LEU B 421	-20.370	70.850	25.418	1.00	46.50	6
	ATOM	1249	CD1	LEU B 421	-20.529	69.890	24.255	1.00	45.15	6
20	ATOM	1250	CD2	LEU B 421	-21.383	70.538	26.486	1.00	51.31	6
	ATOM	1251	C	LEU B 421	-17.547	72.452	24.823	1.00	39.59	6
	ATOM	1252	O	LEU B 421	-17.975	73.035	23.836	1.00	40.66	8
	ATOM	1253	N	LEU B 422	-16.847	73.059	25.780	1.00	39.57	7
	ATOM	1254	CA	LEU B 422	-16.534	74.478	25.715	1.00	38.63	6
25	ATOM	1255	CB	LEU B 422	-15.829	74.936	26.992	1.00	41.79	6
	ATOM	1256	CG	LEU B 422	-16.714	75.149	28.191	1.00	42.74	6
	ATOM	1257	CD1	LEU B 422	-15.911	75.685	29.360	1.00	42.89	6
	ATOM	1258	CD2	LEU B 422	-17.783	76.162	27.813	1.00	39.27	6
	ATOM	1259	C	LEU B 422	-15.677	74.788	24.513	1.00	40.47	6
30	ATOM	1260	O	LEU B 422	-15.823	75.846	23.917	1.00	47.83	8
	ATOM	1261	N	MET B 423	-14.789	73.853	24.168	1.00	34.27	7
	ATOM	1262	CA	MET B 423	-13.907	74.019	23.024	1.00	35.25	6
	ATOM	1263	CB	MET B 423	-12.920	72.858	22.922	1.00	32.56	6
	ATOM	1264	CG	MET B 423	-12.013	72.703	24.125	1.00	40.70	6
35	ATOM	1265	SD	MET B 423	-10.345	72.007	23.784	1.00	47.65	16
	ATOM	1266	CE	MET B 423	-10.770	70.538	22.761	1.00	47.16	6
	ATOM	1267	C	MET B 423	-14.709	74.100	21.738	1.00	35.13	6
	ATOM	1268	O	MET B 423	-14.341	74.807	20.803	1.00	29.85	8
	ATOM	1269	N	LYS B 424	-15.811	73.361	21.704	1.00	31.56	7
40	ATOM	1270	CA	LYS B 424	-16.676	73.354	20.544	1.00	32.29	6
	ATOM	1271	CB	LYS B 424	-17.783	72.316	20.736	1.00	30.56	6
	ATOM	1272	CG	LYS B 424	-17.257	70.879	20.843	1.00	30.07	6
	ATOM	1273	CD	LYS B 424	-16.444	70.510	19.611	1.00	33.22	6
	ATOM	1274	CE	LYS B 424	-15.795	69.136	19.706	1.00	28.75	6
45	ATOM	1275	NZ	LYS B 424	-14.655	69.067	20.678	1.00	31.01	7
	ATOM	1276	C	LYS B 424	-17.248	74.754	20.304	1.00	29.26	6
	ATOM	1277	O	LYS B 424	-17.439	75.149	19.166	1.00	30.22	8
	ATOM	1278	N	VAL B 425	-17.495	75.499	21.385	1.00	23.53	7
	ATOM	1279	CA	VAL B 425	-18.014	76.852	21.278	1.00	28.91	6
50	ATOM	1280	CB	VAL B 425	-18.278	77.458	22.663	1.00	29.44	6
	ATOM	1281	CG1	VAL B 425	-18.633	78.915	22.547	1.00	28.81	6
	ATOM	1282	CG2	VAL B 425	-19.401	76.733	23.354	1.00	31.22	6
	ATOM	1283	C	VAL B 425	-17.001	77.682	20.498	1.00	32.03	6
	ATOM	1284	O	VAL B 425	-17.368	78.465	19.629	1.00	31.95	8
55	ATOM	1285	N	THR B 426	-15.721	77.508	20.827	1.00	33.61	7
	ATOM	1286	CA	THR B 426	-14.645	78.221	20.137	1.00	30.76	6
	ATOM	1287	CB	THR B 426	-13.270	77.912	20.761	1.00	32.34	6
	ATOM	1288	OG1	THR B 426	-13.073	78.697	21.941	1.00	33.07	8



5	ATOM	1289	CG2	THR	B	426	-12.153	78.174	19.782	1.00	25.40	6
	ATOM	1290	C	THR	B	426	-14.677	77.742	18.706	1.00	32.53	6
	ATOM	1291	O	THR	B	426	-14.639	78.530	17.763	1.00	35.19	8
	ATOM	1292	N	ASP	B	427	-14.749	76.425	18.566	1.00	28.83	7
	ATOM	1293	CA	ASP	B	427	-14.796	75.807	17.257	1.00	35.12	6
10	ATOM	1294	CB	ASP	B	427	-15.096	74.302	17.380	1.00	39.14	6
	ATOM	1295	CG	ASP	B	427	-13.910	73.496	17.806	1.00	45.80	6
	ATOM	1296	OD1	ASP	B	427	-12.786	73.774	17.348	1.00	41.97	8
	ATOM	1297	OD2	ASP	B	427	-14.064	72.517	18.583	1.00	50.06	8
	ATOM	1298	C	ASP	B	427	-15.883	76.502	16.429	1.00	33.94	6
15	ATOM	1299	O	ASP	B	427	-15.673	76.815	15.262	1.00	38.02	8
	ATOM	1300	N	LEU	B	428	-17.040	76.741	17.048	1.00	27.15	7
	ATOM	1301	CA	LEU	B	428	-18.154	77.388	16.367	1.00	29.99	6
	ATOM	1302	CB	LEU	B	428	-19.448	77.190	17.168	1.00	22.49	6
	ATOM	1303	CG	LEU	B	428	-20.086	75.818	17.089	1.00	25.54	6
20	ATOM	1304	CD1	LEU	B	428	-21.282	75.729	18.012	1.00	20.60	6
	ATOM	1305	CD2	LEU	B	428	-20.509	75.564	15.651	1.00	17.24	6
	ATOM	1306	C	LEU	B	428	-17.901	78.863	16.103	1.00	28.94	6
	ATOM	1307	O	LEU	B	428	-18.328	79.388	15.076	1.00	31.26	8
	ATOM	1308	N	ARG	B	429	-17.213	79.524	17.035	1.00	27.64	7
25	ATOM	1309	CA	ARG	B	429	-16.894	80.937	16.883	1.00	28.13	6
	ATOM	1310	CB	ARG	B	429	-16.274	81.507	18.160	1.00	29.59	6
	ATOM	1311	CG	ARG	B	429	-17.246	81.752	19.302	1.00	34.85	6
	ATOM	1312	CD	ARG	B	429	-16.626	82.653	20.372	1.00	47.18	6
	ATOM	1313	NE	ARG	B	429	-17.373	82.714	21.620	1.00	57.93	7
30	ATOM	1314	CZ	ARG	B	429	-18.632	83.124	21.716	1.00	63.62	6
	ATOM	1315	NH1	ARG	B	429	-19.263	83.579	20.622	1.00	60.71	7
	ATOM	1316	NH2	ARG	B	429	-19.238	83.130	22.916	1.00	62.38	7
	ATOM	1317	C	ARG	B	429	-15.930	81.146	15.728	1.00	29.81	6
	ATOM	1318	O	ARG	B	429	-16.101	82.061	14.933	1.00	30.81	8
35	ATOM	1319	N	MET	B	430	-14.908	80.295	15.670	1.00	29.64	7
	ATOM	1320	CA	MET	B	430	-13.920	80.343	14.614	1.00	34.72	6
	ATOM	1321	CB	MET	B	430	-12.939	79.192	14.763	1.00	34.97	6
	ATOM	1322	CG	MET	B	430	-11.787	79.431	15.689	1.00	45.34	6
	ATOM	1323	SD	MET	B	430	-10.729	80.768	15.158	1.00	52.55	16
40	ATOM	1324	CE	MET	B	430	-10.070	80.157	13.610	1.00	55.56	6
	ATOM	1325	C	MET	B	430	-14.638	80.217	13.284	1.00	34.01	6
	ATOM	1326	O	MET	B	430	-14.395	80.996	12.385	1.00	37.29	8
	ATOM	1327	N	ILE	B	431	-15.516	79.217	13.176	1.00	29.99	7
	ATOM	1328	CA	ILE	B	431	-16.296	78.992	11.963	1.00	28.82	6
45	ATOM	1329	CB	ILE	B	431	-17.391	77.929	12.177	1.00	27.39	6
	ATOM	1330	CG2	ILE	B	431	-18.314	77.841	10.959	1.00	23.87	6
	ATOM	1331	CG1	ILE	B	431	-16.784	76.555	12.449	1.00	25.56	6
	ATOM	1332	CD1	ILE	B	431	-17.826	75.464	12.498	1.00	17.29	6
	ATOM	1333	C	ILE	B	431	-16.953	80.288	11.538	1.00	29.49	6
50	ATOM	1334	O	ILE	B	431	-16.837	80.725	10.398	1.00	24.19	8
	ATOM	1335	N	GLY	B	432	-17.657	80.904	12.474	1.00	25.25	7
	ATOM	1336	CA	GLY	B	432	-18.357	82.142	12.179	1.00	30.38	6
	ATOM	1337	C	GLY	B	432	-17.395	83.209	11.725	1.00	32.75	6
	ATOM	1338	O	GLY	B	432	-17.531	83.740	10.637	1.00	36.38	8
55	ATOM	1339	N	ALA	B	433	-16.431	83.522	12.586	1.00	26.77	7
	ATOM	1340	CA	ALA	B	433	-15.407	84.514	12.299	1.00	26.48	6
	ATOM	1341	CB	ALA	B	433	-14.240	84.338	13.253	1.00	19.90	6
	ATOM	1342	C	ALA	B	433	-14.905	84.433	10.867	1.00	30.73	6

5	ATOM	1343	O	ALA	B	433	-14.849	85.432	10.171	1.00	31.60	8
	ATOM	1344	N	CYS	B	434	-14.534	83.246	10.439	1.00	33.22	7
	ATOM	1345	CA	CYS	B	434	-14.023	83.021	9.120	1.00	34.34	6
	ATOM	1346	CB	CYS	B	434	-13.553	81.661	9.226	1.00	35.20	6
	ATOM	1347	SG	CYS	B	434	-12.412	81.249	8.444	1.00	54.48	16
10	ATOM	1348	C	CYS	B	434	-15.106	83.116	8.062	1.00	34.09	6
	ATOM	1349	O	CYS	B	434	-14.844	83.555	6.952	1.00	34.89	8
	ATOM	1350	N	HIS	B	435	-16.318	82.699	8.394	1.00	34.30	7
	ATOM	1351	CA	HIS	B	435	-17.395	82.762	7.443	1.00	35.44	6
	ATOM	1352	CB	HIS	B	435	-18.700	82.404	8.103	1.00	31.76	6
15	ATOM	1353	CG	HIS	B	435	-19.845	82.425	7.149	1.00	32.03	6
	ATOM	1354	CD2	HIS	B	435	-20.483	81.419	6.515	1.00	28.61	6
	ATOM	1355	ND1	HIS	B	435	-20.345	83.600	6.607	1.00	28.48	7
	ATOM	1356	CE1	HIS	B	435	-21.241	83.293	5.672	1.00	33.27	6
	ATOM	1357	NE2	HIS	B	435	-21.341	81.977	5.605	1.00	31.57	7
20	ATOM	1358	C	HIS	B	435	-17.528	84.152	6.878	1.00	32.74	6
	ATOM	1359	O	HIS	B	435	-17.842	84.326	5.715	1.00	32.87	8
	ATOM	1360	N	ALA	B	436	-17.315	85.121	7.758	1.00	31.01	7
	ATOM	1361	CA	ALA	B	436	-17.376	86.520	7.405	1.00	29.91	6
	ATOM	1362	CB	ALA	B	436	-17.008	87.352	8.618	1.00	21.23	6
25	ATOM	1363	C	ALA	B	436	-16.393	86.782	6.266	1.00	33.86	6
	ATOM	1364	O	ALA	B	436	-16.734	87.398	5.257	1.00	36.10	8
	ATOM	1365	N	SER	B	437	-15.162	86.307	6.448	1.00	35.19	7
	ATOM	1366	CA	SER	B	437	-14.122	86.484	5.445	1.00	33.03	6
	ATOM	1367	CB	SER	B	437	-12.882	85.688	5.847	1.00	35.31	6
30	ATOM	1368	OG	SER	B	437	-11.855	85.824	4.879	1.00	44.99	8
	ATOM	1369	C	SER	B	437	-14.642	85.993	4.108	1.00	38.39	6
	ATOM	1370	O	SER	B	437	-14.700	86.730	3.127	1.00	37.54	8
	ATOM	1371	N	ARG	B	438	-15.008	84.719	4.096	1.00	37.32	7
	ATOM	1372	CA	ARG	B	438	-15.526	84.068	2.908	1.00	39.30	6
35	ATOM	1373	CB	ARG	B	438	-16.019	82.660	3.259	1.00	42.97	6
	ATOM	1374	CG	ARG	B	438	-14.910	81.673	3.590	1.00	41.72	6
	ATOM	1375	CD	ARG	B	438	-14.044	81.488	2.356	1.00	45.23	6
	ATOM	1376	NE	ARG	B	438	-14.781	80.936	1.235	1.00	45.66	7
	ATOM	1377	CZ	ARG	B	438	-14.482	81.175	-0.040	1.00	49.71	6
40	ATOM	1378	NH1	ARG	B	438	-13.458	81.977	-0.347	1.00	50.91	7
	ATOM	1379	NH2	ARG	B	438	-15.219	80.619	-1.002	1.00	46.86	7
	ATOM	1380	C	ARG	B	438	-16.659	84.859	2.287	1.00	42.37	6
	ATOM	1381	O	ARG	B	438	-16.841	84.832	1.072	1.00	40.58	8
	ATOM	1382	N	PHE	B	439	-17.417	85.575	3.117	1.00	42.25	7
45	ATOM	1383	CA	PHE	B	439	-18.531	86.354	2.614	1.00	42.81	6
	ATOM	1384	CB	PHE	B	439	-19.198	87.132	3.731	1.00	42.18	6
	ATOM	1385	CG	PHE	B	439	-20.487	87.769	3.323	1.00	42.48	6
	ATOM	1386	CD1	PHE	B	439	-21.535	86.981	2.912	1.00	47.09	6
	ATOM	1387	CD2	PHE	B	439	-20.638	89.141	3.334	1.00	39.76	6
50	ATOM	1388	CE1	PHE	B	439	-22.735	87.543	2.527	1.00	49.17	6
	ATOM	1389	CE2	PHE	B	439	-21.851	89.717	2.944	1.00	45.10	6
	ATOM	1390	CZ	PHE	B	439	-22.901	88.911	2.538	1.00	46.36	6
	ATOM	1391	C	PHE	B	439	-18.016	87.319	1.581	1.00	44.79	6
	ATOM	1392	O	PHE	B	439	-18.514	87.354	0.465	1.00	40.26	8
55	ATOM	1393	N	LEU	B	440	-17.021	88.117	1.987	1.00	42.77	7
	ATOM	1394	CA	LEU	B	440	-16.415	89.115	1.109	1.00	42.96	6
	ATOM	1395	CB	LEU	B	440	-15.169	89.718	1.768	1.00	37.19	6
	ATOM	1396	CG	LEU	B	440	-15.477	90.588	2.967	1.00	36.97	6

5	ATOM	1397	CD1	LEU	B	440	-14.219	91.352	3.402	1.00	33.65	6
	ATOM	1398	CD2	LEU	B	440	-16.577	91.591	2.574	1.00	35.42	6
	ATOM	1399	C	LEU	B	440	-16.099	88.561	-0.273	1.00	45.47	6
	ATOM	1400	O	LEU	B	440	-16.631	89.059	-1.265	1.00	52.48	8
	ATOM	1401	N	HIS	B	441	-15.238	87.549	-0.345	1.00	49.15	7
10	ATOM	1402	CA	HIS	B	441	-14.929	86.956	-1.632	1.00	54.76	6
	ATOM	1403	CB	HIS	B	441	-14.150	85.700	-1.448	1.00	56.68	6
	ATOM	1404	CG	HIS	B	441	-12.713	85.934	-1.230	1.00	62.73	6
	ATOM	1405	CD2	HIS	B	441	-11.602	85.418	-1.812	1.00	65.73	6
	ATOM	1406	ND1	HIS	B	441	-12.245	86.850	-0.273	1.00	66.01	7
15	ATOM	1407	CE1	HIS	B	441	-10.916	86.847	-0.309	1.00	65.55	6
	ATOM	1408	NE2	HIS	B	441	-10.512	85.993	-1.228	1.00	60.09	7
	ATOM	1409	C	HIS	B	441	-16.217	86.633	-2.301	1.00	55.93	6
	ATOM	1410	O	HIS	B	441	-16.418	86.938	-3.465	1.00	57.33	8
	ATOM	1411	N	MET	B	442	-17.106	85.997	-1.553	1.00	57.81	7
20	ATOM	1412	CA	MET	B	442	-18.399	85.652	-2.106	1.00	59.11	6
	ATOM	1413	CB	MET	B	442	-19.340	85.162	-1.008	1.00	55.93	6
	ATOM	1414	CG	MET	B	442	-18.991	83.796	-0.456	1.00	58.52	6
	ATOM	1415	SD	MET	B	442	-20.310	82.994	0.505	1.00	60.99	16
	ATOM	1416	CE	MET	B	442	-20.525	84.203	1.827	1.00	52.61	6
25	ATOM	1417	C	MET	B	442	-18.991	86.879	-2.785	1.00	60.31	6
	ATOM	1418	O	MET	B	442	-19.646	86.778	-3.817	1.00	58.18	8
	ATOM	1419	N	LYS	B	443	-18.731	88.045	-2.213	1.00	61.45	7
	ATOM	1420	CA	LYS	B	443	-19.267	89.268	-2.758	1.00	64.90	6
	ATOM	1421	CB	LYS	B	443	-19.182	90.358	-1.704	1.00	64.40	6
30	ATOM	1422	CG	LYS	B	443	-20.160	91.449	-1.982	1.00	69.12	6
	ATOM	1423	CD	LYS	B	443	-19.763	92.673	-1.306	1.00	71.14	6
	ATOM	1424	CE	LYS	B	443	-20.508	92.993	-0.491	1.00	73.43	6
	ATOM	1425	NZ	LYS	B	443	-20.174	94.242	0.151	1.00	67.97	7
	ATOM	1426	C	LYS	B	443	-18.528	89.704	-4.020	1.00	67.29	6
35	ATOM	1427	O	LYS	B	443	-18.979	90.586	-4.731	1.00	67.90	8
	ATOM	1428	N	VAL	B	444	-17.383	89.075	-4.285	1.00	66.57	7
	ATOM	1429	CA	VAL	B	444	-16.589	89.418	-5.455	1.00	64.76	6
	ATOM	1430	CB	VAL	B	444	-15.097	89.568	-5.082	1.00	62.76	6
	ATOM	1431	CG1	VAL	B	444	-14.269	89.857	-6.298	1.00	64.00	6
40	ATOM	1432	CG2	VAL	B	444	-14.905	90.678	-4.042	1.00	59.27	6
	ATOM	1433	C	VAL	B	444	-16.800	88.397	-6.569	1.00	68.61	6
	ATOM	1434	O	VAL	B	444	-16.968	88.774	-7.729	1.00	70.60	8
	ATOM	1435	N	GLU	B	445	-16.812	87.118	-6.219	1.00	70.71	7
	ATOM	1436	CA	GLU	B	445	-16.951	86.033	-7.197	1.00	71.45	6
45	ATOM	1437	CB	GLU	B	445	-16.169	84.809	-6.712	1.00	72.36	6
	ATOM	1438	CG	GLU	B	445	-14.736	85.090	-6.392	1.00	40.00	6
	ATOM	1439	CD	GLU	B	445	-13.998	83.890	-5.851	1.00	40.00	6
	ATOM	1440	OE1	GLU	B	445	-14.587	82.798	-5.665	1.00	40.00	8
	ATOM	1441	OE2	GLU	B	445	-12.775	83.995	-5.580	1.00	40.00	8
50	ATOM	1442	C	GLU	B	445	-18.375	85.574	-7.422	1.00	71.46	6
	ATOM	1443	O	GLU	B	445	-18.605	84.542	-8.064	1.00	73.02	8
	ATOM	1444	N	CYS	B	446	-19.328	86.333	-6.900	1.00	71.12	7
	ATOM	1445	CA	CYS	B	446	-20.694	85.942	-7.062	1.00	70.83	6
	ATOM	1446	CB	CYS	B	446	-21.196	85.230	-5.784	1.00	71.05	6
55	ATOM	1447	SG	CYS	B	446	-20.296	83.720	-5.349	1.00	72.83	16
	ATOM	1448	C	CYS	B	446	-21.563	87.135	-7.386	1.00	71.91	6
	ATOM	1449	O	CYS	B	446	-21.307	88.244	-6.911	1.00	72.06	8
	ATOM	1450	N	PRO	B	447	-22.550	86.928	-8.256	1.00	73.12	7

5	ATOM	1451	CD	PRO B 447	-22.837	85.637	-8.886	1.00	72.88	6
	ATOM	1452	CA	PRO B 447	-23.461	87.997	-8.653	1.00	74.22	6
	ATOM	1453	CB	PRO B 447	-24.399	87.338	-9.659	1.00	72.98	6
	ATOM	1454	CG	PRO B 447	-23.981	85.934	-9.776	1.00	74.77	6
	ATOM	1455	C	PRO B 447	-24.203	88.519	-7.451	1.00	75.94	6
10	ATOM	1456	O	PRO B 447	-24.601	87.749	-6.611	1.00	76.67	8
	ATOM	1457	N	THR B 448	-24.390	89.828	-7.373	1.00	76.91	7
	ATOM	1458	CA	THR B 448	-25.134	90.436	-6.268	1.00	78.24	6
	ATOM	1459	CB	THR B 448	-24.883	91.948	-6.276	1.00	81.33	6
	ATOM	1460	OG1	THR B 448	-25.474	92.525	-7.451	1.00	84.46	8
15	ATOM	1461	CG2	THR B 448	-23.394	92.234	-6.269	1.00	83.51	6
	ATOM	1462	C	THR B 448	-26.594	90.160	-6.619	1.00	77.42	6
	ATOM	1463	O	THR B 448	-27.512	90.649	-5.982	1.00	77.65	8
	ATOM	1464	N	GLU B 449	-26.759	89.400	-7.697	1.00	76.29	7
	ATOM	1465	CA	GLU B 449	-28.051	89.017	-8.211	1.00	75.03	6
20	ATOM	1466	CB	GLU B 449	-27.923	88.915	-9.719	1.00	74.62	6
	ATOM	1467	CG	GLU B 449	-28.823	87.966	-10.343	1.00	40.00	6
	ATOM	1468	CD	GLU B 449	-28.522	87.831	-11.756	1.00	40.00	6
	ATOM	1469	OE1	GLU B 449	-27.366	88.072	-12.190	1.00	40.00	8
	ATOM	1470	OE2	GLU B 449	-29.449	87.438	-12.492	1.00	40.00	8
25	ATOM	1471	C	GLU B 449	-28.448	87.660	-7.609	1.00	73.49	6
	ATOM	1472	O	GLU B 449	-29.479	87.092	-7.953	1.00	70.24	8
	ATOM	1473	N	LEU B 450	-27.624	87.158	-6.695	1.00	70.80	7
	ATOM	1474	CA	LEU B 450	-27.879	85.879	-6.058	1.00	68.82	6
	ATOM	1475	CB	LEU B 450	-26.772	84.887	-6.447	1.00	71.91	6
30	ATOM	1476	CG	LEU B 450	-26.612	84.503	-7.900	1.00	76.62	6
	ATOM	1477	CD1	LEU B 450	-25.396	83.637	-8.059	1.00	77.95	6
	ATOM	1478	CD2	LEU B 450	-27.849	83.775	-8.351	1.00	76.46	6
	ATOM	1479	C	LEU B 450	-27.941	86.012	-4.536	1.00	66.22	6
	ATOM	1480	O	LEU B 450	-28.251	85.039	-3.849	1.00	66.01	8
35	ATOM	1481	N	PHE B 451	-27.666	87.215	-4.012	1.00	61.96	7
	ATOM	1482	CA	PHE B 451	-27.635	87.494	-2.585	1.00	58.44	6
	ATOM	1483	CB	PHE B 451	-26.579	88.573	-2.263	1.00	61.34	6
	ATOM	1484	CG	PHE B 451	-25.153	88.078	-2.413	1.00	63.02	6
	ATOM	1485	CD1	PHE B 451	-24.675	87.587	-3.626	1.00	62.92	6
40	ATOM	1486	CD2	PHE B 451	-24.283	88.173	-1.346	1.00	63.07	6
	ATOM	1487	CE1	PHE B 451	-23.327	87.217	-3.757	1.00	65.12	6
	ATOM	1488	CE2	PHE B 451	-22.939	87.806	-1.472	1.00	64.66	6
	ATOM	1489	CZ	PHE B 451	-22.459	87.335	-2.686	1.00	67.12	6
	ATOM	1490	C	PHE B 451	-28.931	87.994	-1.962	1.00	56.41	6
45	ATOM	1491	O	PHE B 451	-29.207	89.214	-1.908	1.00	56.56	8
	ATOM	1492	N	PRO B 452	-29.791	87.072	-1.473	1.00	53.28	7
	ATOM	1493	CD	PRO B 452	-29.767	85.611	-1.494	1.00	50.46	6
	ATOM	1494	CA	PRO B 452	-31.037	87.598	-0.843	1.00	50.26	6
	ATOM	1495	CB	PRO B 452	-31.746	86.375	-0.301	1.00	49.19	6
50	ATOM	1496	CG	PRO B 452	-31.024	85.197	-0.842	1.00	45.89	6
	ATOM	1497	C	PRO B 452	-30.636	88.567	0.251	1.00	49.62	6
	ATOM	1498	O	PRO B 452	-29.628	88.401	0.906	1.00	52.35	8
	ATOM	1499	N	PRO B 453	-31.494	89.539	0.535	1.00	51.50	7
	ATOM	1500	CD	PRO B 453	-32.853	89.644	0.022	1.00	49.66	6
55	ATOM	1501	CA	PRO B 453	-31.184	90.573	1.530	1.00	50.89	6
	ATOM	1502	CB	PRO B 453	-32.422	91.401	1.625	1.00	51.49	6
	ATOM	1503	CG	PRO B 453	-33.378	90.827	0.724	1.00	50.82	6
	ATOM	1504	C	PRO B 453	-30.829	90.039	2.906	1.00	50.99	6

5	ATOM	1505	O	PRO B 453	-29.700	90.206	3.345	1.00	54.17	8
	ATOM	1506	N	LEU B 454	-31.807	89.458	3.631	1.00	51.21	7
	ATOM	1507	CA	LEU B 454	-31.538	88.945	4.948	1.00	47.17	6
	ATOM	1508	CB	LEU B 454	-32.550	87.858	5.330	1.00	44.44	6
	ATOM	1509	CG	LEU B 454	-32.347	87.412	6.748	1.00	41.33	6
10	ATOM	1510	CD1	LEU B 454	-31.987	88.589	7.631	1.00	35.93	6
	ATOM	1511	CD2	LEU B 454	-33.590	86.732	7.239	1.00	34.79	6
	ATOM	1512	C	LEU B 454	-30.099	88.443	4.928	1.00	42.25	6
	ATOM	1513	O	LEU B 454	-29.323	88.774	5.812	1.00	40.82	8
	ATOM	1514	N	PHE B 455	-29.716	87.707	3.885	1.00	39.29	7
15	ATOM	1515	CA	PHE B 455	-28.347	87.204	3.770	1.00	41.81	6
	ATOM	1516	CB	PHE B 455	-28.132	86.536	2.418	1.00	47.22	6
	ATOM	1517	CG	PHE B 455	-26.813	85.836	2.292	1.00	56.97	6
	ATOM	1518	CD1	PHE B 455	-26.437	84.915	3.247	1.00	57.23	6
	ATOM	1519	CD2	PHE B 455	-25.949	86.094	1.236	1.00	59.40	6
20	ATOM	1520	CE1	PHE B 455	-25.225	84.234	3.153	1.00	56.58	6
	ATOM	1521	CE2	PHE B 455	-24.720	85.409	1.134	1.00	61.80	6
	ATOM	1522	CZ	PHE B 455	-24.360	84.481	2.103	1.00	59.94	6
	ATOM	1523	C	PHE B 455	-27.400	88.386	3.923	1.00	45.12	6
	ATOM	1524	O	PHE B 455	-26.657	88.450	4.889	1.00	39.95	8
25	ATOM	1525	N	LEU B 456	-27.439	89.303	2.949	1.00	43.92	7
	ATOM	1526	CA	LEU B 456	-26.597	90.503	2.947	1.00	44.08	6
	ATOM	1527	CB	LEU B 456	-27.001	91.440	1.802	1.00	50.20	6
	ATOM	1528	CG	LEU B 456	-26.439	91.155	0.432	1.00	55.79	6
	ATOM	1529	CD1	LEU B 456	-27.064	92.082	-0.591	1.00	54.70	6
30	ATOM	1530	CD2	LEU B 456	-24.920	91.345	0.494	1.00	53.01	6
	ATOM	1531	C	LEU B 456	-26.689	91.245	4.264	1.00	44.65	6
	ATOM	1532	O	LEU B 456	-25.678	91.540	4.886	1.00	45.93	8
	ATOM	1533	N	GLU B 457	-27.990	91.268	4.265	1.00	44.56	7
	ATOM	1534	CA	GLU B 457	-28.288	92.016	5.497	1.00	46.37	6
35	ATOM	1535	C	GLU B 457	-27.434	91.452	6.628	1.00	43.60	6
	ATOM	1536	O	GLU B 457	-26.754	92.223	7.339	1.00	42.69	8
	ATOM	1537	CB	GLU B 457	-29.769	91.879	5.855	1.00	50.16	6
	ATOM	1538	CG	GLU B 457	-30.208	92.849	6.954	1.00	20.00	6
	ATOM	1539	CD	GLU B 457	-31.646	93.338	6.782	1.00	20.00	6
40	ATOM	1540	OE1	GLU B 457	-32.351	92.932	5.779	1.00	20.00	8
	ATOM	1541	OE2	GLU B 457	-32.157	94.156	7.638	1.00	20.00	8
	ATOM	1542	N	VAL B 458	-27.428	90.413	7.281	1.00	43.21	7
	ATOM	1543	CA	VAL B 458	-26.706	89.739	8.351	1.00	44.98	6
	ATOM	1544	CB	VAL B 458	-27.075	88.255	8.432	1.00	44.83	6
45	ATOM	1545	CG1	VAL B 458	-26.440	87.623	9.646	1.00	49.72	6
	ATOM	1546	CG2	VAL B 458	-28.562	88.086	8.474	1.00	40.89	6
	ATOM	1547	C	VAL B 458	-25.190	89.822	8.311	1.00	42.72	6
	ATOM	1548	O	VAL B 458	-24.551	90.179	9.303	1.00	42.88	8
	ATOM	1549	N	PHE B 459	-24.605	89.488	7.180	1.00	44.53	7
50	ATOM	1550	CA	PHE B 459	-23.165	89.480	7.077	1.00	48.18	6
	ATOM	1551	CB	PHE B 459	-22.747	88.457	6.065	1.00	43.60	6
	ATOM	1552	CG	PHE B 459	-23.167	87.116	6.441	1.00	40.79	6
	ATOM	1553	CD1	PHE B 459	-24.494	86.750	6.368	1.00	41.01	6
	ATOM	1554	CD2	PHE B 459	-22.263	86.286	7.009	1.00	39.48	6
55	ATOM	1555	CE1	PHE B 459	-24.892	85.540	6.889	1.00	40.62	6
	ATOM	1556	CE2	PHE B 459	-22.649	85.091	7.527	1.00	36.87	6
	ATOM	1557	CZ	PHE B 459	-23.967	84.711	7.455	1.00	36.39	6
	ATOM	1558	C	PHE B 459	-22.627	90.758	6.623	1.00	52.71	6

5	ATOM	1559	O	PHE	B	459	-21.414	91.050	6.791	1.00	51.34	8
	ATOM	1560	N	GLU	B	460	-23.489	91.531	5.976	1.00	62.92	7
	ATOM	1561	CA	GLU	B	460	-22.953	92.741	5.533	1.00	69.33	6
	ATOM	1562	CB	GLU	B	460	-23.851	93.487	4.505	1.00	72.95	6
	ATOM	1563	CG	GLU	B	460	-22.917	94.002	3.412	1.00	78.35	6
10	ATOM	1564	CD	GLU	B	460	-22.908	95.480	3.256	1.00	82.97	6
	ATOM	1565	OE1	GLU	B	460	-23.257	96.213	4.217	1.00	88.28	8
	ATOM	1566	OE2	GLU	B	460	-22.524	95.977	2.167	1.00	84.80	8
	ATOM	1567	C	GLU	B	460	-22.790	93.576	6.786	1.00	71.87	6
	ATOM	1568	O	GLU	B	460	-23.471	93.391	7.802	1.00	74.51	8
15	ATOM	1569	N	ASP	B	461	-21.796	94.449	6.696	1.00	78.50	7
	ATOM	1570	CA	ASP	B	461	-21.401	95.328	7.701	1.00	84.19	6
	ATOM	1571	CB	ASP	B	461	-20.182	96.032	7.125	1.00	85.82	6
	ATOM	1572	CG	ASP	B	461	-19.261	95.066	6.463	1.00	89.62	6
	ATOM	1573	OD1	ASP	B	461	-19.670	93.929	5.982	1.00	93.00	8
20	ATOM	1574	OD2	ASP	B	461	-18.084	95.361	6.387	1.00	93.04	8
	ATOM	1575	C	ASP	B	461	-22.540	96.291	8.012	1.00	86.80	6
	ATOM	1576	O	ASP	B	461	-23.063	96.176	9.139	1.00	88.70	8
	ATOM	1577	OXT	ASP	B	461	-22.962	97.048	7.098	1.00	88.70	8
	TER											
25	ATOM	4002	C1	T3	J	1	20.152	36.643	29.561	1.00	22.34	6
	ATOM	4003	C2	T3	J	1	19.021	41.567	29.283	1.00	21.84	6
	ATOM	4004	C3	T3	J	1	18.880	37.086	29.226	1.00	23.43	6
	ATOM	4005	C4	T3	J	1	18.249	42.606	28.776	1.00	22.31	6
	ATOM	4006	C5	T3	J	1	18.747	38.372	28.866	1.00	24.83	6
30	ATOM	4007	C6	T3	J	1	17.938	43.621	29.664	1.00	25.16	6
	ATOM	4008	C7	T3	J	1	19.799	39.296	28.753	1.00	24.65	6
	ATOM	4009	C8	T3	J	1	18.330	43.594	31.028	1.00	21.93	6
	ATOM	4010	C9	T3	J	1	21.101	38.940	29.075	1.00	25.09	6
	ATOM	4011	C10	T3	J	1	19.063	42.558	31.465	1.00	23.66	6
35	ATOM	4012	C11	T3	J	1	21.254	37.600	29.456	1.00	23.12	6
	ATOM	4013	C12	T3	J	1	19.459	41.490	30.621	1.00	19.67	6
	ATOM	4014	C13	T3	J	1	20.370	35.228	30.075	1.00	18.97	6
	ATOM	4015	C15	T3	J	1	21.549	34.480	29.455	1.00	19.32	6
	ATOM	4016	C17	T3	J	1	21.535	33.003	29.710	1.00	19.02	6
40	ATOM	4017	I1	T3	J	1	16.898	39.029	28.661	1.00	25.29	53
	ATOM	4018	I2	T3	J	1	17.058	45.327	29.154	1.00	26.49	53
	ATOM	4019	I3	T3	J	1	22.763	40.262	29.169	1.00	25.67	53
	ATOM	4020	N1	T3	J	1	21.800	34.859	28.024	1.00	15.12	7
	ATOM	4021	O1	T3	J	1	17.934	44.682	31.806	1.00	21.79	8
45	ATOM	4022	O2	T3	J	1	19.432	40.560	28.362	1.00	22.05	8
	ATOM	4023	O3	T3	J	1	21.911	32.260	28.776	1.00	20.38	8
	ATOM	4024	O4	T3	J	1	21.137	32.622	30.840	1.00	20.16	8
	TER											
	ATOM	4025	C1	T3	K	1	-28.131	75.928	7.543	1.00	22.34	6
50	ATOM	4026	C2	T3	K	1	-24.676	77.673	4.318	1.00	21.84	6
	ATOM	4027	C3	T3	K	1	-28.490	76.351	6.201	1.00	23.43	6
	ATOM	4028	C4	T3	K	1	-24.217	77.893	2.989	1.00	22.31	6
	ATOM	4029	C5	T3	K	1	-27.485	76.499	5.233	1.00	24.83	6
	ATOM	4030	C6	T3	K	1	-23.545	79.124	2.700	1.00	25.16	6
55	ATOM	4031	C7	T3	K	1	-26.132	76.227	5.581	1.00	24.65	6
	ATOM	4032	C8	T3	K	1	-23.382	80.104	3.772	1.00	21.93	6
	ATOM	4033	C9	T3	K	1	-25.685	75.833	6.855	1.00	25.09	6
	ATOM	4034	C10	T3	K	1	-23.867	79.823	5.042	1.00	23.66	6

5	ATOM	4035	C11	T3	K	1	-26.708	75.670	7.834	1.00	23.12	6
	ATOM	4036	C12	T3	K	1	-24.521	78.610	5.376	1.00	19.67	6
	ATOM	4037	C13	T3	K	1	-29.211	75.830	8.626	1.00	18.97	6
	ATOM	4038	C15	T3	K	1	-29.181	74.567	9.488	1.00	19.32	6
	ATOM	4039	C17	T3	K	1	-30.440	74.343	10.264	1.00	19.02	6
10	ATOM	4040	I1	T3	K	1	-27.868	77.342	3.316	1.00	25.29	53
	ATOM	4041	I2	T3	K	1	-22.732	79.619	0.850	1.00	26.49	53
	ATOM	4042	I3	T3	K	1	-23.602	75.792	7.334	1.00	25.67	53
	ATOM	4043	N1	T3	K	1	-28.680	73.342	8.762	1.00	15.12	7
	ATOM	4044	O1	T3	K	1	-22.742	81.265	3.443	1.00	21.79	8
15	ATOM	4045	O2	T3	K	1	-25.267	76.388	4.595	1.00	22.05	8
	ATOM	4046	O3	T3	K	1	-30.816	73.159	10.382	1.00	20.38	8
	ATOM	4047	O4	T3	K	1	-31.028	75.359	10.729	1.00	20.16	8
	TER											
	ATOM	1	C	LYS	X	686	13.868	40.176	48.888	1.00	40.00	6
20	ATOM	2	O	LYS	X	686	13.914	40.120	47.639	1.00	40.00	8
	ATOM	3	N	LYS	X	686	14.374	42.245	50.489	1.00	40.00	7
	ATOM	4	CA	LYS	X	686	14.937	41.070	49.710	1.00	40.00	6
	ATOM	5	N	HIS	X	687	13.038	39.527	49.705	1.00	40.00	7
	ATOM	6	CA	HIS	X	687	11.891	38.518	49.521	1.00	40.00	6
25	ATOM	7	CB	HIS	X	687	10.639	39.000	50.212	1.00	40.00	6
	ATOM	8	CG	HIS	X	687	10.981	39.526	51.563	1.00	40.00	6
	ATOM	9	CD2	HIS	X	687	11.021	38.908	52.753	1.00	40.00	6
	ATOM	10	ND1	HIS	X	687	11.354	40.844	51.754	1.00	40.00	7
	ATOM	11	CE1	HIS	X	687	11.614	40.994	53.034	1.00	40.00	6
30	ATOM	12	NE2	HIS	X	687	11.422	39.847	53.646	1.00	40.00	7
	ATOM	13	C	HIS	X	687	11.183	38.108	48.208	1.00	40.00	6
	ATOM	14	O	HIS	X	687	11.674	38.361	47.094	1.00	40.00	8
	ATOM	15	N	LYS	X	688	10.064	37.458	48.649	1.00	40.00	7
	ATOM	16	CA	LYS	X	688	8.911	36.858	47.931	1.00	40.00	6
35	ATOM	17	CB	LYS	X	688	8.292	37.850	46.968	1.00	40.00	6
	ATOM	18	C	LYS	X	688	9.246	35.573	47.161	1.00	40.00	6
	ATOM	19	O	LYS	X	688	9.319	34.473	47.722	1.00	40.00	8
	ATOM	20	N	ILE	X	689	9.426	35.754	45.865	1.00	40.00	7
	ATOM	21	CA	ILE	X	689	9.661	34.640	44.924	1.00	40.00	6
40	ATOM	22	CB	ILE	X	689	9.731	35.167	43.498	1.00	40.00	6
	ATOM	23	CG2	ILE	X	689	9.638	34.053	42.453	1.00	40.00	6
	ATOM	24	CG1	ILE	X	689	8.597	36.141	43.176	1.00	40.00	6
	ATOM	25	CD1	ILE	X	689	8.250	36.183	41.688	1.00	40.00	6
	ATOM	26	C	ILE	X	689	10.954	33.869	45.228	1.00	40.00	6
45	ATOM	27	O	ILE	X	689	10.920	32.657	45.511	1.00	40.00	8
	ATOM	28	N	LEU	X	690	12.065	34.579	45.140	1.00	40.00	7
	ATOM	29	CA	LEU	X	690	13.391	33.996	45.397	1.00	40.00	6
	ATOM	30	CB	LEU	X	690	14.349	35.043	45.892	1.00	40.00	6
	ATOM	31	CG	LEU	X	690	14.450	36.168	44.906	1.00	40.00	6
50	ATOM	32	CD1	LEU	X	690	15.397	37.261	45.363	1.00	40.00	6
	ATOM	33	CD2	LEU	X	690	14.940	35.695	43.540	1.00	40.00	6
	ATOM	34	C	LEU	X	690	13.271	32.999	46.466	1.00	40.00	6
	ATOM	35	O	LEU	X	690	13.633	31.832	46.315	1.00	40.00	8
	ATOM	36	N	HIS	X	691	12.773	33.472	47.541	1.00	40.00	7
55	ATOM	37	CA	HIS	X	691	12.557	32.559	48.569	1.00	40.00	6
	ATOM	38	CB	HIS	X	691	11.729	33.212	49.658	1.00	40.00	6
	ATOM	39	CG	HIS	X	691	12.588	34.116	50.564	1.00	40.00	6
	ATOM	40	CD2	HIS	X	691	13.648	33.852	51.385	1.00	40.00	6

5	ATOM	41	ND1	HIS	X	691	12.359	35.484	50.669	1.00	40.00	7
	ATOM	42	CE1	HIS	X	691	13.242	35.991	51.513	1.00	40.00	6
	ATOM	43	NE2	HIS	X	691	14.016	35.031	51.949	1.00	40.00	7
	ATOM	44	C	HIS	X	691	11.954	31.331	47.861	1.00	40.00	6
	ATOM	45	O	HIS	X	691	12.505	30.240	47.882	1.00	40.00	8
10	ATOM	46	N	ARG	X	692	10.839	31.494	47.167	1.00	40.00	7
	ATOM	47	CA	ARG	X	692	10.169	30.333	46.518	1.00	40.00	6
	ATOM	48	CB	ARG	X	692	9.118	30.800	45.517	1.00	40.00	6
	ATOM	49	C	ARG	X	692	11.153	29.402	45.752	1.00	40.00	6
	ATOM	50	O	ARG	X	692	11.030	28.168	45.779	1.00	40.00	8
15	ATOM	51	N	LEU	X	693	12.117	30.000	45.072	1.00	40.00	7
	ATOM	52	CA	LEU	X	693	13.078	29.252	44.226	1.00	40.00	6
	ATOM	53	CB	LEU	X	693	13.784	30.210	43.274	1.00	40.00	6
	ATOM	54	CG	LEU	X	693	12.796	31.012	42.432	1.00	40.00	6
	ATOM	55	CD1	LEU	X	693	13.479	31.969	41.458	1.00	40.00	6
20	ATOM	56	CD2	LEU	X	693	11.884	30.126	41.579	1.00	40.00	6
	ATOM	57	C	LEU	X	693	14.143	28.531	45.054	1.00	40.00	6
	ATOM	58	O	LEU	X	693	14.702	27.508	44.633	1.00	40.00	8
	ATOM	59	N	LEU	X	694	14.400	29.079	46.209	1.00	40.00	7
	ATOM	60	CA	LEU	X	694	15.407	28.538	47.115	1.00	40.00	6
25	ATOM	61	CB	LEU	X	694	15.871	29.626	48.084	1.00	40.00	6
	ATOM	62	CG	LEU	X	694	16.692	30.716	47.404	1.00	40.00	6
	ATOM	63	CD1	LEU	X	694	17.279	31.724	48.391	1.00	40.00	6
	ATOM	64	CD2	LEU	X	694	17.879	30.156	46.619	1.00	40.00	6
	ATOM	65	C	LEU	X	694	14.837	27.404	47.957	1.00	40.00	6
30	ATOM	66	O	LEU	X	694	15.555	26.747	48.716	1.00	40.00	8
	ATOM	67	N	GLN	X	695	13.554	27.157	47.809	1.00	40.00	7
	ATOM	68	CA	GLN	X	695	12.883	26.188	48.685	1.00	40.00	6
	ATOM	69	C	GLN	X	695	12.423	24.910	47.977	1.00	40.00	6
	ATOM	70	O	GLN	X	695	12.309	23.845	48.598	1.00	40.00	8
35	ATOM	71	CB	GLN	X	695	11.681	26.858	49.322	1.00	40.00	6
	ATOM	72	CG	GLN	X	695	12.074	28.125	50.080	1.00	20.00	6
	ATOM	73	CD	GLN	X	695	10.899	28.768	50.801	1.00	20.00	6
	ATOM	74	OE1	GLN	X	695	9.772	28.296	50.671	1.00	20.00	8
	ATOM	75	NE2	GLN	X	695	11.092	29.828	51.560	1.00	20.00	7
40	ATOM	76	N	ASP	X	696	12.155	25.020	46.714	1.00	40.00	7
	ATOM	77	CA	ASP	X	696	11.698	23.885	45.910	1.00	40.00	6
	ATOM	78	CB	ASP	X	696	11.450	24.400	44.497	1.00	40.00	6
	ATOM	79	CG	ASP	X	696	10.782	23.411	43.548	1.00	40.00	6
	ATOM	80	OD1	ASP	X	696	10.550	22.203	43.920	1.00	40.00	8
45	ATOM	81	OD2	ASP	X	696	10.449	23.804	42.362	1.00	40.00	8
	ATOM	82	C	ASP	X	696	12.774	22.806	45.876	1.00	40.00	6
	ATOM	83	O	ASP	X	696	13.937	23.077	45.562	1.00	40.00	8
	ATOM	84	N	SER	X	697	12.370	21.610	46.213	1.00	40.00	7
	ATOM	85	CA	SER	X	697	13.258	20.453	46.128	1.00	40.00	6
50	ATOM	86	CB	SER	X	697	12.685	19.371	47.049	1.00	40.00	6
	ATOM	87	OG	SER	X	697	12.535	19.899	48.374	1.00	40.00	8
	ATOM	88	C	SER	X	697	13.329	20.130	44.613	1.00	40.00	6
	ATOM	89	O	SER	X	697	14.247	20.573	43.914	1.00	40.00	8
	ATOM	90	N	SER	X	698	12.355	19.357	44.183	1.00	40.00	7
55	ATOM	91	CA	SER	X	698	11.985	19.100	42.752	1.00	40.00	6
	ATOM	92	CB	SER	X	698	11.693	20.417	42.036	1.00	40.00	6
	ATOM	93	OG	SER	X	698	10.510	21.000	42.577	1.00	40.00	8
	ATOM	94	C	SER	X	698	12.887	18.340	41.758	1.00	40.00	6



5	ATOM	95	O	SER	X	698	13.253	17.158	42.026	1.00	40.00	8
	ATOM	96	OXT	SER	X	698	13.131	18.976	40.714	1.00	40.00	8
	TER											
	ATOM	1	CB	LYS	Y	688	-33.793	96.885	6.491	1.00	40.00	6
	ATOM	2	C	LYS	Y	688	-35.002	95.370	8.130	1.00	40.00	6
10	ATOM	3	O	LYS	Y	688	-36.027	95.520	8.779	1.00	40.00	8
	ATOM	4	N	LYS	Y	688	-32.717	96.619	8.695	1.00	40.00	7
	ATOM	5	CA	LYS	Y	688	-34.040	96.591	7.954	1.00	40.00	6
	ATOM	6	N	ILE	Y	689	-34.578	93.781	6.908	1.00	40.00	7
	ATOM	7	CA	ILE	Y	689	-35.862	93.106	7.268	1.00	40.00	6
15	ATOM	8	CB	ILE	Y	689	-35.971	91.759	6.572	1.00	40.00	6
	ATOM	9	CG2	ILE	Y	689	-37.270	91.077	6.932	1.00	40.00	6
	ATOM	10	CG1	ILE	Y	689	-35.917	91.937	5.062	1.00	40.00	6
	ATOM	11	CD1	ILE	Y	689	-36.341	90.691	4.289	1.00	40.00	6
	ATOM	12	C	ILE	Y	689	-36.032	92.870	8.780	1.00	40.00	6
20	ATOM	13	O	ILE	Y	689	-36.913	93.446	9.442	1.00	40.00	8
	ATOM	14	N	LEU	Y	690	-35.019	92.834	9.787	1.00	40.00	7
	ATOM	15	CA	LEU	Y	690	-34.956	92.320	11.163	1.00	40.00	6
	ATOM	16	CB	LEU	Y	690	-33.528	92.432	11.697	1.00	40.00	6
	ATOM	17	CG	LEU	Y	690	-32.516	91.647	10.864	1.00	40.00	6
25	ATOM	18	CD1	LEU	Y	690	-31.087	91.764	11.397	1.00	40.00	6
	ATOM	19	CD2	LEU	Y	690	-32.819	90.148	10.812	1.00	40.00	6
	ATOM	20	C	LEU	Y	690	-35.899	93.123	12.065	1.00	40.00	6
	ATOM	21	O	LEU	Y	690	-36.570	92.492	12.928	1.00	40.00	8
	ATOM	22	N	HIS	Y	691	-36.039	94.731	11.373	1.00	40.00	7
30	ATOM	23	CA	HIS	Y	691	-36.634	94.923	12.683	1.00	40.00	6
	ATOM	24	CB	HIS	Y	691	-36.354	96.383	12.935	1.00	40.00	6
	ATOM	25	CG	HIS	Y	691	-35.610	97.153	13.078	1.00	40.00	6
	ATOM	26	CD2	HIS	Y	691	-34.757	97.640	12.159	1.00	40.00	6
	ATOM	27	ND1	HIS	Y	691	-35.129	97.579	14.319	1.00	40.00	7
35	ATOM	28	CE1	HIS	Y	691	-34.039	98.290	14.122	1.00	40.00	6
	ATOM	29	NE2	HIS	Y	691	-33.786	98.346	12.815	1.00	40.00	7
	ATOM	30	C	HIS	Y	691	-37.972	94.287	12.756	1.00	40.00	6
	ATOM	31	O	HIS	Y	691	-38.240	93.417	13.545	1.00	40.00	8
	ATOM	32	N	ARG	Y	692	-38.265	94.388	11.505	1.00	40.00	7
40	ATOM	33	CA	ARG	Y	692	-39.577	93.869	11.276	1.00	40.00	6
	ATOM	34	CB	ARG	Y	692	-39.653	93.692	9.795	1.00	40.00	6
	ATOM	35	CG	ARG	Y	692	-40.759	92.764	9.329	1.00	40.00	6
	ATOM	36	CD	ARG	Y	692	-40.618	92.422	7.848	1.00	40.00	6
	ATOM	37	NE	ARG	Y	692	-41.849	92.641	7.091	1.00	40.00	7
45	ATOM	38	CZ	ARG	Y	692	-41.898	92.758	5.763	1.00	40.00	6
	ATOM	39	NH1	ARG	Y	692	-40.784	92.695	5.024	1.00	40.00	7
	ATOM	40	NH2	ARG	Y	692	-43.034	92.940	5.080	1.00	40.00	7
	ATOM	41	C	ARG	Y	692	-39.941	92.547	11.995	1.00	40.00	6
	ATOM	42	O	ARG	Y	692	-41.001	92.440	12.649	1.00	40.00	8
50	ATOM	43	N	LEU	Y	693	-39.095	91.576	11.816	1.00	40.00	7
	ATOM	44	CA	LEU	Y	693	-39.230	90.232	12.395	1.00	40.00	6
	ATOM	45	CB	LEU	Y	693	-38.362	89.337	11.615	1.00	40.00	6
	ATOM	46	CG	LEU	Y	693	-38.737	89.375	10.132	1.00	40.00	6
	ATOM	47	CD1	LEU	Y	693	-37.794	88.570	9.247	1.00	40.00	6
55	ATOM	48	CD2	LEU	Y	693	-40.142	88.827	9.862	1.00	40.00	6
	ATOM	49	C	LEU	Y	693	-38.921	90.378	13.816	1.00	40.00	6
	ATOM	50	O	LEU	Y	693	-39.191	89.474	14.615	1.00	40.00	8
	ATOM	51	N	LEU	Y	694	-38.366	91.533	14.076	1.00	40.00	7

5	ATOM	52	CA	LEU	Y	694	-38.174	91.885	15.435	1.00	40.00	6
	ATOM	53	CB	LEU	Y	694	-37.181	93.002	15.561	1.00	40.00	6
	ATOM	54	CG	LEU	Y	694	-35.799	92.377	15.869	1.00	40.00	6
	ATOM	55	CD1	LEU	Y	694	-34.897	93.275	16.702	1.00	40.00	6
	ATOM	56	CD2	LEU	Y	694	-35.897	91.055	16.661	1.00	40.00	6
10	ATOM	57	C	LEU	Y	694	-39.596	91.903	15.915	1.00	40.00	6
	ATOM	58	O	LEU	Y	694	-39.985	91.253	16.858	1.00	40.00	8
	ATOM	59	N	GLN	Y	695	-40.787	92.229	15.048	1.00	40.00	7
	ATOM	60	CA	GLN	Y	695	-42.034	91.457	15.543	1.00	40.00	6
	ATOM	61	C	GLN	Y	695	-43.054	90.901	14.240	1.00	40.00	6
15	ATOM	62	O	GLN	Y	695	-43.102	91.557	13.189	1.00	40.00	8
	ATOM	63	CB	GLN	Y	695	-42.362	92.025	16.923	1.00	40.00	6
	ATOM	64	CG	GLN	Y	695	-41.013	92.101	17.768	1.00	40.00	6
	ATOM	65	CD	GLN	Y	695	-40.943	91.235	19.059	1.00	40.00	6
	ATOM	66	OE1	GLN	Y	695	-41.828	90.426	19.318	1.00	40.00	8
20	ATOM	67	NE2	GLN	Y	695	-39.938	91.399	19.916	1.00	40.00	7
	ATOM	68	N	ASP	Y	696	-43.802	89.498	14.402	1.00	40.00	7
	ATOM	69	CA	ASP	Y	696	-44.784	88.354	13.428	1.00	40.00	6
	ATOM	70	C	ASP	Y	696	-46.034	88.934	12.759	1.00	40.00	6
	ATOM	71	O	ASP	Y	696	-46.266	88.655	11.529	1.00	40.00	8
25	ATOM	72	CB	ASP	Y	696	-45.211	87.192	14.322	1.00	40.00	6
	ATOM	73	CG	ASP	Y	696	-44.021	86.560	15.058	1.00	40.00	6
	ATOM	74	OD1	ASP	Y	696	-42.823	86.994	14.844	1.00	40.00	8
	ATOM	75	OD2	ASP	Y	696	-44.212	85.591	15.889	1.00	40.00	8
	END											
30												

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## Appendix 2

Atomic Coordinates for Human ER $\alpha$  Complexed with DES, and a GRIP1 NR-box 2 Peptide

10	CRYST1	54.094	82.217	58.041	90.00	111.33	90.00	P	21	2	
	ORIGX1	1.000000	0.000000	0.000000	0.000000						
	ORIGX2	0.000000	1.000000	0.000000	0.000000						
	ORIGX3	0.000000	0.000000	1.000000	0.000000						
	SCALE1	0.018486	0.000000	0.007221	0.000000						
15	SCALE2	0.000000	0.012163	0.000000	0.000000						
	SCALE3	0.000000	0.000000	0.018497	0.000000						
	ATOM	1	CB	SER	A	305	35.230	-14.787	-1.163	1.00	73.26
	ATOM	2	C	SER	A	305	35.331	-14.303	1.289	1.00	72.95
20	ATOM	3	O	SER	A	305	34.146	-13.984	1.186	1.00	72.46
	ATOM	4	N	SER	A	305	36.797	-16.033	0.285	1.00	74.06
	ATOM	5	CA	SER	A	305	36.138	-14.713	0.061	1.00	73.59
	ATOM	6	N	LEU	A	306	35.982	-14.313	2.449	1.00	72.21
	ATOM	7	CA	LEU	A	306	35.329	-13.950	3.702	1.00	71.05
25	ATOM	8	CB	LEU	A	306	36.251	-14.256	4.878	1.00	70.19
	ATOM	9	C	LEU	A	306	34.929	-12.478	3.719	1.00	69.57
	ATOM	10	O	LEU	A	306	35.580	-11.638	3.100	1.00	69.96
	ATOM	11	N	ALA	A	307	33.851	-12.176	4.434	1.00	68.06
	ATOM	12	CA	ALA	A	307	33.358	-10.810	4.541	1.00	64.88
30	ATOM	13	CB	ALA	A	307	31.841	-10.795	4.436	1.00	65.83
	ATOM	14	C	ALA	A	307	33.792	-10.204	5.866	1.00	63.36
	ATOM	15	O	ALA	A	307	33.878	-8.984	6.005	1.00	62.73
	ATOM	16	N	LEU	A	308	34.064	-11.062	6.842	1.00	62.52
	ATOM	17	CA	LEU	A	308	34.487	-10.598	8.156	1.00	62.57
35	ATOM	18	CB	LEU	A	308	34.423	-11.745	9.171	1.00	62.81
	ATOM	19	CG	LEU	A	308	33.214	-12.688	9.130	1.00	64.21
	ATOM	20	CD1	LEU	A	308	33.188	-13.513	10.406	1.00	66.28
	ATOM	21	CD2	LEU	A	308	31.919	-11.898	8.989	1.00	63.80
	ATOM	22	C	LEU	A	308	35.903	-10.037	8.100	1.00	61.61
40	ATOM	23	O	LEU	A	308	36.385	-9.445	9.066	1.00	62.92
	ATOM	24	N	SER	A	309	36.561	-10.219	6.959	1.00	60.50
	ATOM	25	CA	SER	A	309	37.928	-9.743	6.771	1.00	58.73
	ATOM	26	CB	SER	A	309	38.720	-10.750	5.934	1.00	59.53
	ATOM	27	OG	SER	A	309	38.889	-10.283	4.606	1.00	59.47
45	ATOM	28	C	SER	A	309	37.986	-8.373	6.099	1.00	57.05
	ATOM	29	O	SER	A	309	38.965	-7.637	6.249	1.00	56.70
	ATOM	30	N	LEU	A	310	36.940	-8.038	5.352	1.00	52.69
	ATOM	31	CA	LEU	A	310	36.877	-6.759	4.658	1.00	48.20
	ATOM	32	CB	LEU	A	310	35.516	-6.596	3.974	1.00	48.32
50	ATOM	33	CG	LEU	A	310	35.301	-7.188	2.583	1.00	44.94
	ATOM	34	CD1	LEU	A	310	33.951	-6.728	2.055	1.00	46.45
	ATOM	35	CD2	LEU	A	310	36.417	-6.755	1.650	1.00	43.19
	ATOM	36	C	LEU	A	310	37.086	-5.589	5.609	1.00	46.44
	ATOM	37	O	LEU	A	310	36.605	-5.607	6.741	1.00	46.78
55	ATOM	38	N	THR	A	311	37.812	-4.576	5.148	1.00	44.36
	ATOM	39	CA	THR	A	311	38.034	-3.380	5.949	1.00	42.88
	ATOM	40	CB	THR	A	311	39.313	-2.633	5.532	1.00	42.31
	ATOM	41	OG1	THR	A	311	39.079	-1.936	4.303	1.00	42.50
	ATOM	42	CG2	THR	A	311	40.464	-3.606	5.350	1.00	46.02
60	ATOM	43	C	THR	A	311	36.834	-2.475	5.674	1.00	43.21

5	ATOM	44	O	THR	A	311	36.021	-2.776	4.800	1.00	42.12
	ATOM	45	N	ALA	A	312	36.726	-1.372	6.409	1.00	42.16
	ATOM	46	CA	ALA	A	312	35.616	-0.444	6.228	1.00	40.10
	ATOM	47	CB	ALA	A	312	35.741	0.709	7.205	1.00	40.07
	ATOM	48	C	ALA	A	312	35.561	0.090	4.799	1.00	41.80
10	ATOM	49	O	ALA	A	312	34.510	0.074	4.154	1.00	37.81
	ATOM	50	N	ASP	A	313	36.698	0.564	4.304	1.00	42.35
	ATOM	51	CA	ASP	A	313	36.752	1.104	2.953	1.00	42.27
	ATOM	52	CB	ASP	A	313	38.133	1.703	2.680	1.00	43.74
	ATOM	53	CG	ASP	A	313	38.323	3.054	3.348	1.00	46.62
15	ATOM	54	OD1	ASP	A	313	39.414	3.645	3.205	1.00	51.01
	ATOM	55	OD2	ASP	A	313	37.380	3.529	4.015	1.00	48.89
	ATOM	56	C	ASP	A	313	36.422	0.027	1.926	1.00	38.68
	ATOM	57	O	ASP	A	313	35.704	0.281	0.959	1.00	38.75
	ATOM	58	N	GLN	A	314	36.931	-1.179	2.145	1.00	34.76
20	ATOM	59	CA	GLN	A	314	36.666	-2.277	1.229	1.00	33.55
	ATOM	60	CB	GLN	A	314	37.462	-3.512	1.643	1.00	36.90
	ATOM	61	CG	GLN	A	314	38.963	-3.384	1.436	1.00	40.45
	ATOM	62	CD	GLN	A	314	39.700	-4.610	1.905	1.00	43.13
	ATOM	63	OE1	GLN	A	314	39.394	-5.196	2.935	1.00	43.60
25	ATOM	64	NE2	GLN	A	314	40.701	-5.032	1.117	1.00	44.03
	ATOM	65	C	GLN	A	314	35.176	-2.595	1.201	1.00	34.95
	ATOM	66	O	GLN	A	314	34.605	-2.860	0.140	1.00	32.89
	ATOM	67	N	MET	A	315	34.542	-2.564	2.374	1.00	32.54
	ATOM	68	CA	MET	A	315	33.115	-2.848	2.470	1.00	35.46
30	ATOM	69	CB	MET	A	315	32.650	-2.794	3.926	1.00	37.09
	ATOM	70	CG	MET	A	315	31.137	-2.777	4.097	1.00	39.42
	ATOM	71	SD	MET	A	315	30.443	-4.426	4.053	1.00	46.55
	ATOM	72	CE	MET	A	315	31.351	-5.205	5.397	1.00	45.29
	ATOM	73	C	MET	A	315	32.311	-1.859	1.640	1.00	31.83
35	ATOM	74	O	MET	A	315	31.453	-2.247	0.852	1.00	32.10
	ATOM	75	N	VAL	A	316	32.587	-0.560	1.830	1.00	32.62
	ATOM	76	CA	VAL	A	316	31.882	0.470	1.079	1.00	31.09
	ATOM	77	CB	VAL	A	316	32.395	1.888	1.425	1.00	34.77
	ATOM	78	CG1	VAL	A	316	31.786	2.899	0.461	1.00	34.10
40	ATOM	79	CG2	VAL	A	316	32.021	2.246	2.862	1.00	34.40
	ATOM	80	C	VAL	A	316	32.092	0.232	-0.414	1.00	33.48
	ATOM	81	O	VAL	A	316	31.145	0.266	-1.200	1.00	32.49
	ATOM	82	N	SER	A	317	33.337	-0.027	-0.795	1.00	33.49
	ATOM	83	CA	SER	A	317	33.682	-0.280	-2.187	1.00	32.88
45	ATOM	84	CB	SER	A	317	35.165	-0.635	-2.297	1.00	35.77
	ATOM	85	OG	SER	A	317	35.825	0.277	-3.154	1.00	42.70
	ATOM	86	C	SER	A	317	32.849	-1.396	-2.801	1.00	30.71
	ATOM	87	O	SER	A	317	32.279	-1.238	-3.880	1.00	31.14
	ATOM	88	N	ALA	A	318	32.792	-2.529	-2.111	1.00	29.51
50	ATOM	89	CA	ALA	A	318	32.035	-3.676	-2.580	1.00	29.93
	ATOM	90	CB	ALA	A	318	32.156	-4.811	-1.579	1.00	28.56
	ATOM	91	C	ALA	A	318	30.565	-3.305	-2.771	1.00	31.55
	ATOM	92	O	ALA	A	318	29.961	-3.642	-3.784	1.00	30.64
	ATOM	93	N	LEU	A	319	29.997	-2.614	-1.791	1.00	34.13
55	ATOM	94	CA	LEU	A	319	28.597	-2.212	-1.861	1.00	32.93
	ATOM	95	CB	LEU	A	319	28.170	-1.576	-0.540	1.00	31.15
	ATOM	96	CG	LEU	A	319	28.076	-2.555	0.632	1.00	32.27
	ATOM	97	CD1	LEU	A	319	27.523	-1.840	1.852	1.00	32.14
	ATOM	98	CD2	LEU	A	319	27.194	-3.733	0.243	1.00	31.82
60	ATOM	99	C	LEU	A	319	28.340	-1.257	-3.020	1.00	34.41
	ATOM	100	O	LEU	A	319	27.430	-1.475	-3.818	1.00	35.23

5	ATOM	101	N	LEU	A	320	29.140	-0.195	-3.120	1.00	32.53
	ATOM	102	CA	LEU	A	320	28.972	0.756	-4.212	1.00	35.33
	ATOM	103	CB	LEU	A	320	30.052	1.839	-4.155	1.00	33.52
	ATOM	104	CG	LEU	A	320	29.974	2.899	-3.054	1.00	34.60
	ATOM	105	CD1	LEU	A	320	31.060	3.940	-3.292	1.00	33.69
10	ATOM	106	CD2	LEU	A	320	28.611	3.562	-3.044	1.00	31.05
	ATOM	107	C	LEU	A	320	29.052	0.040	-5.561	1.00	35.41
	ATOM	108	O	LEU	A	320	28.230	0.271	-6.446	1.00	39.16
	ATOM	109	N	AASP	A	321	30.042	-0.833	-5.720	0.50	36.33
	ATOM	110	N	BASP	A	321	30.041	-0.839	-5.695	0.50	35.76
15	ATOM	111	CA	AASP	A	321	30.214	-1.559	-6.977	0.50	37.71
	ATOM	112	CA	BASP	A	321	30.258	-1.595	-6.925	0.50	37.11
	ATOM	113	CB	AASP	A	321	31.537	-2.334	-6.973	0.50	40.01
	ATOM	114	CB	BASP	A	321	31.573	-2.374	-6.826	0.50	39.41
	ATOM	115	CG	AASP	A	321	31.694	-3.230	-8.195	0.50	41.93
20	ATOM	116	CG	BASP	A	321	32.770	-1.562	-7.284	0.50	39.96
	ATOM	117	OD1	AASP	A	321	31.523	-2.733	-9.329	0.50	42.11
	ATOM	118	OD1	BASP	A	321	33.312	-1.868	-8.366	0.50	43.41
	ATOM	119	OD2	AASP	A	321	31.988	-4.432	-8.022	0.50	42.69
	ATOM	120	OD2	BASP	A	321	33.170	-0.622	-6.564	0.50	41.33
25	ATOM	121	C	AASP	A	321	29.069	-2.524	-7.275	0.50	37.19
	ATOM	122	C	BASP	A	321	29.123	-2.565	-7.253	0.50	36.68
	ATOM	123	O	AASP	A	321	28.820	-2.861	-8.434	0.50	36.87
	ATOM	124	O	BASP	A	321	28.934	-2.942	-8.411	0.50	36.08
	ATOM	125	N	ALA	A	322	28.374	-2.968	-6.235	1.00	35.35
30	ATOM	126	CA	ALA	A	322	27.268	-3.902	-6.417	1.00	31.59
	ATOM	127	CB	ALA	A	322	27.124	-4.781	-5.175	1.00	30.73
	ATOM	128	C	ALA	A	322	25.946	-3.204	-6.709	1.00	30.07
	ATOM	129	O	ALA	A	322	24.955	-3.857	-7.036	1.00	26.53
	ATOM	130	N	GLU	A	323	25.932	-1.880	-6.596	1.00	27.98
35	ATOM	131	CA	GLU	A	323	24.713	-1.117	-6.827	1.00	29.88
	ATOM	132	CB	GLU	A	323	25.027	0.380	-6.855	1.00	30.98
	ATOM	133	CG	GLU	A	323	24.870	1.068	-5.509	1.00	31.62
	ATOM	134	CD	GLU	A	323	23.463	0.940	-4.960	1.00	31.98
	ATOM	135	OE1	GLU	A	323	23.183	-0.056	-4.257	1.00	33.10
40	ATOM	136	OE2	GLU	A	323	22.640	1.836	-5.233	1.00	30.01
	ATOM	137	C	GLU	A	323	24.010	-1.515	-8.123	1.00	30.86
	ATOM	138	O	GLU	A	323	24.655	-1.705	-9.151	1.00	28.86
	ATOM	139	N	PRO	A	324	22.674	-1.659	-8.083	1.00	30.66
	ATOM	140	CD	PRO	A	324	21.774	-1.466	-6.935	1.00	31.01
45	ATOM	141	CA	PRO	A	324	21.935	-2.032	-9.290	1.00	30.29
	ATOM	142	CB	PRO	A	324	20.613	-2.598	-8.760	1.00	31.42
	ATOM	143	CG	PRO	A	324	20.626	-2.363	-7.258	1.00	33.66
	ATOM	144	C	PRO	A	324	21.717	-0.785	-10.138	1.00	27.46
	ATOM	145	O	PRO	A	324	21.893	0.332	-9.668	1.00	26.19
50	ATOM	146	N	PRO	A	325	21.335	-0.959	-11.403	1.00	27.80
	ATOM	147	CD	PRO	A	325	21.082	-2.198	-12.161	1.00	27.35
	ATOM	148	CA	PRO	A	325	21.125	0.242	-12.211	1.00	25.59
	ATOM	149	CB	PRO	A	325	21.258	-0.266	-13.637	1.00	24.02
	ATOM	150	CG	PRO	A	325	20.773	-1.695	-13.559	1.00	26.00
55	ATOM	151	C	PRO	A	325	19.749	0.830	-11.954	1.00	23.73
	ATOM	152	O	PRO	A	325	18.873	0.165	-11.402	1.00	24.83
	ATOM	153	N	ILE	A	326	19.571	2.081	-12.352	1.00	22.11
	ATOM	154	CA	ILE	A	326	18.296	2.762	-12.212	1.00	24.01
	ATOM	155	CB	ILE	A	326	18.502	4.282	-12.133	1.00	25.97
60	ATOM	156	CG2	ILE	A	326	17.168	4.992	-12.286	1.00	20.75
	ATOM	157	CG1	ILE	A	326	19.189	4.632	-10.805	1.00	29.31

5	ATOM	158	CD1	ILE	A	326	19.301	6.120-10.525	1.00	32.91
	ATOM	159	C	ILE	A	326	17.506	2.408-13.471	1.00	25.72
	ATOM	160	O	ILE	A	326	17.906	2.758-14.581	1.00	25.55
10	ATOM	161	N	LEU	A	327	16.392	1.703-13.301	1.00	25.57
	ATOM	162	CA	LEU	A	327	15.595	1.279-14.439	1.00	23.80
	ATOM	163	CB	LEU	A	327	14.872	-0.029-14.104	1.00	23.96
	ATOM	164	CG	LEU	A	327	15.778	-1.210-13.728	1.00	19.89
	ATOM	165	CD1	LEU	A	327	14.944	-2.462-13.583	1.00	21.19
	ATOM	166	CD2	LEU	A	327	16.850	-1.415-14.805	1.00	17.53
15	ATOM	167	C	LEU	A	327	14.598	2.317-14.935	1.00	27.16
	ATOM	168	O	LEU	A	327	14.161	3.202-14.194	1.00	25.98
	ATOM	169	N	TYR	A	328	14.251	2.207-16.210	1.00	26.56
	ATOM	170	CA	TYR	A	328	13.303	3.123-16.814	1.00	24.45
	ATOM	171	CB	TYR	A	328	13.724	3.465-18.245	1.00	26.72
	ATOM	172	CG	TYR	A	328	14.587	4.693-18.314	1.00	27.73
20	ATOM	173	CD1	TYR	A	328	14.021	5.949-18.518	1.00	28.56
	ATOM	174	CE1	TYR	A	328	14.798	7.092-18.509	1.00	29.10
	ATOM	175	CD2	TYR	A	328	15.962	4.612-18.110	1.00	26.01
	ATOM	176	CE2	TYR	A	328	16.750	5.753-18.098	1.00	30.63
	ATOM	177	CZ	TYR	A	328	16.157	6.988-18.297	1.00	30.07
	ATOM	178	OH	TYR	A	328	16.917	8.130-18.265	1.00	37.94
25	ATOM	179	C	TYR	A	328	11.923	2.501-16.827	1.00	24.95
	ATOM	180	O	TYR	A	328	11.774	1.274-16.846	1.00	27.02
	ATOM	181	N	SER	A	329	10.912	3.358-16.800	1.00	25.60
	ATOM	182	CA	SER	A	329	9.533	2.908-16.837	1.00	29.45
	ATOM	183	CB	SER	A	329	8.661	3.858-16.020	1.00	30.80
	ATOM	184	OG	SER	A	329	7.297	3.721-16.364	1.00	33.74
30	ATOM	185	C	SER	A	329	9.129	2.947-18.313	1.00	31.30
	ATOM	186	O	SER	A	329	9.908	3.397-19.154	1.00	27.35
	ATOM	187	N	GLU	A	330	7.930	2.469-18.629	1.00	32.98
	ATOM	188	CA	GLU	A	330	7.459	2.482-20.007	1.00	35.10
	ATOM	189	CB	GLU	A	330	6.031	1.968-20.074	1.00	34.67
	ATOM	190	C	GLU	A	330	7.532	3.924-20.505	1.00	40.06
35	ATOM	191	O	GLU	A	330	7.068	4.841-19.826	1.00	42.65
	ATOM	192	N	TYR	A	331	8.124	4.126-21.681	1.00	41.16
	ATOM	193	CA	TYR	A	331	8.263	5.470-22.234	1.00	42.66
	ATOM	194	CB	TYR	A	331	9.323	5.482-23.350	1.00	42.54
	ATOM	195	CG	TYR	A	331	9.202	4.347-24.345	1.00	38.67
	ATOM	196	CD1	TYR	A	331	10.105	3.284-24.334	1.00	34.66
40	ATOM	197	CE1	TYR	A	331	9.985	2.228-25.233	1.00	34.89
	ATOM	198	CD2	TYR	A	331	8.174	4.327-25.287	1.00	37.88
	ATOM	199	CE2	TYR	A	331	8.045	3.276-26.193	1.00	34.65
	ATOM	200	CZ	TYR	A	331	8.950	2.232-26.159	1.00	30.73
	ATOM	201	OH	TYR	A	331	8.814	1.191-27.042	1.00	30.97
	ATOM	202	C	TYR	A	331	6.943	6.043-22.754	1.00	46.24
45	ATOM	203	O	TYR	A	331	6.018	5.301-23.096	1.00	45.38
	ATOM	204	N	ASP	A	332	6.868	7.372-22.792	1.00	49.11
	ATOM	205	CA	ASP	A	332	5.684	8.092-23.262	1.00	52.40
	ATOM	206	CB	ASP	A	332	5.781	8.321-24.772	1.00	52.86
	ATOM	207	C	ASP	A	332	4.356	7.410-22.926	1.00	52.90
	ATOM	208	O	ASP	A	332	3.561	7.116-23.818	1.00	53.94
50	ATOM	209	N	PRO	A	333	4.103	7.144-21.632	1.00	53.63
	ATOM	210	CD	PRO	A	333	4.962	7.418-20.465	1.00	53.63
	ATOM	211	CA	PRO	A	333	2.840	6.497-21.253	1.00	53.55
	ATOM	212	CB	PRO	A	333	3.070	6.076-19.802	1.00	53.78
	ATOM	213	CG	PRO	A	333	4.101	7.028-19.290	1.00	53.42
	ATOM	214	C	PRO	A	333	1.673	7.478-21.398	1.00	52.17

5	ATOM	215	O	PRO	A	333	1.879	8.690-21.395	1.00	51.19
	ATOM	216	N	THR	A	334	0.457	6.956-21.532	1.00	52.26
	ATOM	217	CA	THR	A	334	-0.724	7.802-21.687	1.00	54.21
	ATOM	218	CB	THR	A	334	-1.997	6.949-21.813	1.00	53.90
	ATOM	219	OG1	THR	A	334	-1.971	6.256-23.065	1.00	53.92
10	ATOM	220	CG2	THR	A	334	-3.237	7.821-21.761	1.00	54.15
	ATOM	221	C	THR	A	334	-0.864	8.782-20.525	1.00	56.34
	ATOM	222	O	THR	A	334	-1.389	8.443-19.461	1.00	56.44
	ATOM	223	N	ARG	A	335	-0.386	10.002-20.766	1.00	58.24
	ATOM	224	CA	ARG	A	335	-0.377	11.099-19.801	1.00	57.96
15	ATOM	225	CB	ARG	A	335	-0.569	12.427-20.531	1.00	60.22
	ATOM	226	C	ARG	A	335	-1.349	10.996-18.627	1.00	56.61
	ATOM	227	O	ARG	A	335	-0.919	10.908-17.475	1.00	60.70
	ATOM	228	N	PRO	A	336	-2.667	11.015-18.889	1.00	52.43
	ATOM	229	CD	PRO	A	336	-3.389	11.117-20.165	1.00	49.06
20	ATOM	230	CA	PRO	A	336	-3.587	10.915-17.752	1.00	49.58
	ATOM	231	CB	PRO	A	336	-4.911	11.456-18.302	1.00	48.66
	ATOM	232	CG	PRO	A	336	-4.645	11.809-19.760	1.00	51.33
	ATOM	233	C	PRO	A	336	-3.698	9.468-17.279	1.00	49.25
	ATOM	234	O	PRO	A	336	-4.340	8.644-17.929	1.00	48.06
25	ATOM	235	N	PHE	A	337	-3.063	9.170-16.147	1.00	47.90
	ATOM	236	CA	PHE	A	337	-3.055	7.821-15.582	1.00	46.61
	ATOM	237	CB	PHE	A	337	-2.063	7.732-14.421	1.00	47.73
	ATOM	238	CG	PHE	A	337	-0.649	8.011-14.805	1.00	46.27
	ATOM	239	CD1	PHE	A	337	-0.017	9.168-14.368	1.00	46.55
30	ATOM	240	CD2	PHE	A	337	0.061	7.113-15.591	1.00	48.12
	ATOM	241	CE1	PHE	A	337	1.305	9.429-14.707	1.00	48.09
	ATOM	242	CE2	PHE	A	337	1.386	7.364-15.938	1.00	47.57
	ATOM	243	CZ	PHE	A	337	2.009	8.525-15.495	1.00	48.40
	ATOM	244	C	PHE	A	337	-4.401	7.338-15.071	1.00	46.15
35	ATOM	245	O	PHE	A	337	-5.250	8.127-14.671	1.00	48.34
	ATOM	246	N	SER	A	338	-4.573	6.022-15.080	1.00	45.06
	ATOM	247	CA	SER	A	338	-5.781	5.385-14.578	1.00	45.12
	ATOM	248	CB	SER	A	338	-6.477	4.594-15.684	1.00	44.49
	ATOM	249	OG	SER	A	338	-6.227	3.206-15.554	1.00	45.78
40	ATOM	250	C	SER	A	338	-5.292	4.439-13.488	1.00	47.04
	ATOM	251	O	SER	A	338	-4.090	4.186-13.387	1.00	44.08
	ATOM	252	N	GLU	A	339	-6.206	3.916-12.676	1.00	45.63
	ATOM	253	CA	GLU	A	339	-5.802	3.012-11.608	1.00	45.40
	ATOM	254	CB	GLU	A	339	-7.015	2.521-10.814	1.00	45.66
45	ATOM	255	CG	GLU	A	339	-6.637	1.680 -9.600	1.00	46.81
	ATOM	256	CD	GLU	A	339	-7.717	1.652 -8.535	1.00	47.56
	ATOM	257	OE1	GLU	A	339	-8.471	0.656 -8.477	1.00	47.37
	ATOM	258	OE2	GLU	A	339	-7.810	2.625 -7.754	1.00	49.29
	ATOM	259	C	GLU	A	339	-5.040	1.821-12.170	1.00	45.23
50	ATOM	260	O	GLU	A	339	-3.862	1.641-11.872	1.00	46.51
	ATOM	261	N	ALA	A	340	-5.712	1.010-12.982	1.00	42.87
	ATOM	262	CA	ALA	A	340	-5.078	-0.158-13.574	1.00	40.24
	ATOM	263	CB	ALA	A	340	-6.055	-0.871-14.496	1.00	41.40
	ATOM	264	C	ALA	A	340	-3.837	0.273-14.350	1.00	38.83
55	ATOM	265	O	ALA	A	340	-2.909	-0.515-14.543	1.00	35.58
	ATOM	266	N	SER	A	341	-3.836	1.535-14.773	1.00	35.79
	ATOM	267	CA	SER	A	341	-2.742	2.133-15.537	1.00	36.58
	ATOM	268	CB	SER	A	341	-3.231	3.454-16.154	1.00	39.01
	ATOM	269	OG	SER	A	341	-2.211	4.130-16.864	1.00	36.09
60	ATOM	270	C	SER	A	341	-1.480	2.376-14.691	1.00	35.63
	ATOM	271	O	SER	A	341	-0.389	1.913-15.038	1.00	33.20

5	ATOM	272	N	MET	A	342	-1.626	3.115-13.595	1.00	35.92
	ATOM	273	CA	MET	A	342	-0.498	3.396-12.708	1.00	35.88
	ATOM	274	CB	MET	A	342	-0.912	4.396-11.623	1.00	35.96
	ATOM	275	CG	MET	A	342	0.241	5.218-11.059	1.00	38.02
	ATOM	276	SD	MET	A	342	-0.308	6.374 -9.780	1.00	44.73
10	ATOM	277	CE	MET	A	342	0.626	7.815-10.205	1.00	42.49
	ATOM	278	C	MET	A	342	-0.011	2.100-12.059	1.00	34.17
	ATOM	279	O	MET	A	342	1.195	1.880-11.909	1.00	33.40
	ATOM	280	N	MET	A	343	-0.957	1.243-11.687	1.00	29.95
	ATOM	281	CA	MET	A	343	-0.640	-0.034-11.062	1.00	31.96
15	ATOM	282	CB	MET	A	343	-1.921	-0.810-10.751	1.00	31.70
	ATOM	283	CG	MET	A	343	-2.667	-0.337 -9.502	1.00	37.13
	ATOM	284	SD	MET	A	343	-1.749	-0.507 -7.940	1.00	36.00
	ATOM	285	CE	MET	A	343	-1.468	-2.299 -7.886	1.00	32.14
	ATOM	286	C	MET	A	343	0.234	-0.875-11.979	1.00	31.72
20	ATOM	287	O	MET	A	343	1.159	-1.558-11.527	1.00	30.26
	ATOM	288	N	GLY	A	344	-0.069	-0.823-13.272	1.00	29.04
	ATOM	289	CA	GLY	A	344	0.688	-1.591-14.242	1.00	24.94
	ATOM	290	C	GLY	A	344	2.104	-1.085-14.396	1.00	26.01
	ATOM	291	O	GLY	A	344	3.046	-1.873-14.463	1.00	28.72
25	ATOM	292	N	LEU	A	345	2.257	0.232-14.471	1.00	26.97
	ATOM	293	CA	LEU	A	345	3.576	0.839-14.608	1.00	31.15
	ATOM	294	CB	LEU	A	345	3.459	2.361-14.753	1.00	30.06
	ATOM	295	CG	LEU	A	345	2.765	2.924-15.995	1.00	33.50
	ATOM	296	CD1	LEU	A	345	2.901	4.439-15.999	1.00	33.52
30	ATOM	297	CD2	LEU	A	345	3.379	2.324-17.257	1.00	33.22
	ATOM	298	C	LEU	A	345	4.433	0.534-13.383	1.00	30.31
	ATOM	299	O	LEU	A	345	5.564	0.061-13.505	1.00	32.80
	ATOM	300	N	LEU	A	346	3.884	0.813-12.205	1.00	27.83
	ATOM	301	CA	LEU	A	346	4.595	0.596-10.947	1.00	26.19
35	ATOM	302	CB	LEU	A	346	3.729	1.063 -9.783	1.00	24.51
	ATOM	303	CG	LEU	A	346	3.483	2.569 -9.682	1.00	26.33
	ATOM	304	CD1	LEU	A	346	2.623	2.844 -8.463	1.00	27.33
	ATOM	305	CD2	LEU	A	346	4.809	3.317 -9.587	1.00	24.89
	ATOM	306	C	LEU	A	346	5.032	-0.848-10.707	1.00	25.72
40	ATOM	307	O	LEU	A	346	6.181	-1.102-10.345	1.00	29.86
	ATOM	308	N	THR	A	347	4.117	-1.793-10.891	1.00	23.80
	ATOM	309	CA	THR	A	347	4.436	-3.196-10.674	1.00	23.91
	ATOM	310	CB	THR	A	347	3.164	-4.058-10.641	1.00	26.39
	ATOM	311	OG1	THR	A	347	2.421	-3.860-11.849	1.00	24.57
45	ATOM	312	CG2	THR	A	347	2.301	-3.682 -9.444	1.00	23.98
	ATOM	313	C	THR	A	347	5.366	-3.734-11.756	1.00	26.17
	ATOM	314	O	THR	A	347	6.176	-4.622-11.496	1.00	27.44
	ATOM	315	N	ASN	A	348	5.242	-3.197-12.970	1.00	25.48
	ATOM	316	CA	ASN	A	348	6.092	-3.617-14.082	1.00	23.77
50	ATOM	317	CB	ASN	A	348	5.657	-2.926-15.385	1.00	24.59
	ATOM	318	CG	ASN	A	348	6.522	-3.302-16.571	1.00	29.93
	ATOM	319	OD1	ASN	A	348	7.616	-2.799-16.771	1.00	24.81
	ATOM	320	ND2	ASN	A	348	6.010	-4.236-17.391	1.00	32.61
	ATOM	321	C	ASN	A	348	7.532	-3.229-13.741	1.00	22.82
55	ATOM	322	O	ASN	A	348	8.453	-4.027-13.870	1.00	18.83
	ATOM	323	N	LEU	A	349	7.711	-1.993-13.288	1.00	22.58
	ATOM	324	CA	LEU	A	349	9.030	-1.507-12.914	1.00	21.85
	ATOM	325	CB	LEU	A	349	8.929	-0.028-12.536	1.00	22.00
	ATOM	326	CG	LEU	A	349	10.155	0.673-11.953	1.00	23.64
60	ATOM	327	CD1	LEU	A	349	11.224	0.826-13.017	1.00	19.35
	ATOM	328	CD2	LEU	A	349	9.726	2.040-11.415	1.00	21.97



5	ATOM	329	C	LEU	A	349	9.564	-2.335-11.734	1.00	22.94
	ATOM	330	O	LEU	A	349	10.724	-2.749-11.717	1.00	23.97
	ATOM	331	N	ALA	A	350	8.705	-2.591-10.756	1.00	21.67
	ATOM	332	CA	ALA	A	350	9.113	-3.356 -9.586	1.00	21.83
	ATOM	333	CB	ALA	A	350	7.963	-3.441 -8.593	1.00	18.95
10	ATOM	334	C	ALA	A	350	9.568	-4.757 -9.985	1.00	21.90
	ATOM	335	O	ALA	A	350	10.625	-5.221 -9.554	1.00	24.15
	ATOM	336	N	ASP	A	351	8.767	-5.423-10.810	1.00	23.24
	ATOM	337	CA	ASP	A	351	9.093	-6.772-11.259	1.00	25.87
	ATOM	338	CB	ASP	A	351	8.028	-7.274-12.239	1.00	27.03
15	ATOM	339	CG	ASP	A	351	8.103	-8.772-12.458	1.00	31.64
	ATOM	340	OD1	ASP	A	351	8.217	-9.196-13.628	1.00	35.06
	ATOM	341	OD2	ASP	A	351	8.049	-9.525-11.464	1.00	36.86
	ATOM	342	C	ASP	A	351	10.469	-6.825-11.912	1.00	22.36
	ATOM	343	O	ASP	A	351	11.219	-7.773-11.702	1.00	25.15
20	ATOM	344	N	ARG	A	352	10.810	-5.808-12.697	1.00	23.58
	ATOM	345	CA	ARG	A	352	12.115	-5.787-13.347	1.00	21.07
	ATOM	346	CB	ARG	A	352	12.120	-4.785-14.507	1.00	21.02
	ATOM	347	CG	ARG	A	352	11.539	-5.352-15.797	1.00	20.44
	ATOM	348	CD	ARG	A	352	11.554	-4.319-16.915	1.00	20.43
25	ATOM	349	NE	ARG	A	352	10.592	-3.245-16.687	1.00	19.85
	ATOM	350	CZ	ARG	A	352	10.910	-1.954-16.641	1.00	19.69
	ATOM	351	NH1	ARG	A	352	12.172	-1.564-16.813	1.00	17.36
	ATOM	352	NH2	ARG	A	352	9.962	-1.049-16.441	1.00	21.88
	ATOM	353	C	ARG	A	352	13.223	-5.442-12.350	1.00	22.11
30	ATOM	354	O	ARG	A	352	14.346	-5.945-12.454	1.00	24.13
	ATOM	355	N	GLU	A	353	12.909	-4.587-11.383	1.00	18.66
	ATOM	356	CA	GLU	A	353	13.888	-4.206-10.376	1.00	19.08
	ATOM	357	CB	GLU	A	353	13.317	-3.102 -9.483	1.00	21.62
	ATOM	358	CG	GLU	A	353	13.295	-1.718-10.114	1.00	20.97
35	ATOM	359	CD	GLU	A	353	12.832	-0.648 -9.129	1.00	23.84
	ATOM	360	OE1	GLU	A	353	11.611	-0.531 -8.926	1.00	24.76
	ATOM	361	OE2	GLU	A	353	13.686	0.066 -8.557	1.00	24.95
	ATOM	362	C	GLU	A	353	14.246	-5.423 -9.512	1.00	20.14
	ATOM	363	O	GLU	A	353	15.398	-5.600 -9.104	1.00	19.40
40	ATOM	364	N	LEU	A	354	13.246	-6.257 -9.235	1.00	19.54
	ATOM	365	CA	LEU	A	354	13.434	-7.452 -8.415	1.00	21.77
	ATOM	366	CB	LEU	A	354	12.107	-8.209 -8.270	1.00	23.09
	ATOM	367	CG	LEU	A	354	11.160	-7.606 -7.223	1.00	25.00
	ATOM	368	CD1	LEU	A	354	9.720	-8.013 -7.510	1.00	23.49
45	ATOM	369	CD2	LEU	A	354	11.584	-8.069 -5.839	1.00	23.31
	ATOM	370	C	LEU	A	354	14.500	-8.386 -8.981	1.00	23.21
	ATOM	371	O	LEU	A	354	15.255	-9.007 -8.234	1.00	22.44
	ATOM	372	N	VAL	A	355	14.560	-8.490-10.302	1.00	22.52
	ATOM	373	CA	VAL	A	355	15.551	-9.343-10.935	1.00	21.66
50	ATOM	374	CB	VAL	A	355	15.353	-9.365-12.466	1.00	24.35
	ATOM	375	CG1	VAL	A	355	16.435	-10.214-13.119	1.00	28.16
	ATOM	376	CG2	VAL	A	355	13.957	-9.886-12.798	1.00	21.59
	ATOM	377	C	VAL	A	355	16.944	-8.811-10.606	1.00	23.74
	ATOM	378	O	VAL	A	355	17.857	-9.581-10.291	1.00	23.51
55	ATOM	379	N	HIS	A	356	17.105	-7.489-10.669	1.00	21.27
	ATOM	380	CA	HIS	A	356	18.392	-6.861-10.369	1.00	21.31
	ATOM	381	CB	HIS	A	356	18.384	-5.390-10.811	1.00	19.87
	ATOM	382	CG	HIS	A	356	18.494	-5.205-12.295	1.00	21.77
	ATOM	383	CD2	HIS	A	356	17.543	-5.048-13.248	1.00	21.66
60	ATOM	384	ND1	HIS	A	356	19.704	-5.177-12.955	1.00	21.11
	ATOM	385	CE1	HIS	A	356	19.496	-5.011-14.249	1.00	24.96

5	ATOM	386	NE2	HIS	A	356	18.192	-4.931	-14.455	1.00	18.37
	ATOM	387	C	HIS	A	356	18.702	-6.947	-8.875	1.00	21.41
	ATOM	388	O	HIS	A	356	19.864	-7.111	-8.465	1.00	21.88
	ATOM	389	N	MET	A	357	17.660	-6.843	-8.058	1.00	21.84
	ATOM	390	CA	MET	A	357	17.837	-6.906	-6.610	1.00	21.51
10	ATOM	391	CB	MET	A	357	16.503	-6.668	-5.898	1.00	17.60
	ATOM	392	CG	MET	A	357	16.629	-6.579	-4.369	1.00	19.36
	ATOM	393	SD	MET	A	357	15.051	-6.755	-3.531	1.00	23.64
	ATOM	394	CE	MET	A	357	14.189	-5.332	-4.163	1.00	23.13
	ATOM	395	C	MET	A	357	18.411	-8.259	-6.192	1.00	23.69
15	ATOM	396	O	MET	A	357	19.337	-8.328	-5.389	1.00	24.41
	ATOM	397	N	ILE	A	358	17.856	-9.331	-6.746	1.00	27.14
	ATOM	398	CA	ILE	A	358	18.314	-10.672	-6.425	1.00	28.79
	ATOM	399	CB	ILE	A	358	17.529	-11.725	-7.232	1.00	32.42
	ATOM	400	CG2	ILE	A	358	18.267	-13.064	-7.220	1.00	32.77
20	ATOM	401	CG1	ILE	A	358	16.125	-11.880	-6.644	1.00	31.94
	ATOM	402	CD1	ILE	A	358	15.062	-12.196	-7.680	1.00	34.85
	ATOM	403	C	ILE	A	358	19.801	-10.802	-6.728	1.00	28.75
	ATOM	404	O	ILE	A	358	20.569	-11.305	-5.912	1.00	31.60
	ATOM	405	N	ASN	A	359	20.207	-10.325	-7.897	1.00	27.91
25	ATOM	406	CA	ASN	A	359	21.601	-10.401	-8.293	1.00	29.16
	ATOM	407	CB	ASN	A	359	21.721	-10.172	-9.801	1.00	31.88
	ATOM	408	CG	ASN	A	359	21.253	-11.381	-10.599	1.00	39.34
	ATOM	409	OD1	ASN	A	359	21.916	-12.422	-10.612	1.00	41.27
	ATOM	410	ND2	ASN	A	359	20.102	-11.255	-11.253	1.00	38.58
30	ATOM	411	C	ASN	A	359	22.476	-9.436	-7.510	1.00	30.75
	ATOM	412	O	ASN	A	359	23.686	-9.629	-7.412	1.00	33.35
	ATOM	413	N	TRP	A	360	21.872	-8.400	-6.940	1.00	30.07
	ATOM	414	CA	TRP	A	360	22.634	-7.451	-6.132	1.00	27.87
	ATOM	415	CB	TRP	A	360	21.849	-6.150	-5.948	1.00	24.80
35	ATOM	416	CG	TRP	A	360	22.196	-5.392	-4.691	1.00	23.04
	ATOM	417	CD2	TRP	A	360	21.501	-5.443	-3.438	1.00	19.83
	ATOM	418	CE2	TRP	A	360	22.147	-4.543	-2.564	1.00	22.31
	ATOM	419	CE3	TRP	A	360	20.392	-6.165	-2.972	1.00	20.09
	ATOM	420	CD1	TRP	A	360	23.212	-4.488	-4.529	1.00	18.99
40	ATOM	421	NE1	TRP	A	360	23.187	-3.974	-3.255	1.00	21.17
	ATOM	422	CZ2	TRP	A	360	21.721	-4.340	-1.243	1.00	20.43
	ATOM	423	CZ3	TRP	A	360	19.968	-5.965	-1.661	1.00	20.12
	ATOM	424	CH2	TRP	A	360	20.635	-5.057	-0.812	1.00	18.54
	ATOM	425	C	TRP	A	360	22.892	-8.099	-4.766	1.00	24.88
45	ATOM	426	O	TRP	A	360	23.978	-7.980	-4.198	1.00	25.00
	ATOM	427	N	ALA	A	361	21.879	-8.789	-4.252	1.00	24.08
	ATOM	428	CA	ALA	A	361	21.972	-9.462	-2.958	1.00	26.06
	ATOM	429	CB	ALA	A	361	20.676	-10.203	-2.672	1.00	20.27
	ATOM	430	C	ALA	A	361	23.161	-10.433	-2.897	1.00	28.44
50	ATOM	431	O	ALA	A	361	23.843	-10.531	-1.876	1.00	28.95
	ATOM	432	N	LYS	A	362	23.414	-11.144	-3.992	1.00	31.41
	ATOM	433	CA	LYS	A	362	24.530	-12.097	-4.047	1.00	33.33
	ATOM	434	CB	LYS	A	362	24.564	-12.824	-5.390	1.00	34.81
	ATOM	435	CG	LYS	A	362	23.319	-13.608	-5.756	1.00	36.27
55	ATOM	436	CD	LYS	A	362	23.458	-14.178	-7.167	1.00	38.30
	ATOM	437	CE	LYS	A	362	22.369	-15.193	-7.472	1.00	40.94
	ATOM	438	NZ	LYS	A	362	22.111	-15.322	-8.937	1.00	42.49
	ATOM	439	C	LYS	A	362	25.854	-11.351	-3.893	1.00	34.17
	ATOM	440	O	LYS	A	362	26.880	-11.977	-3.595	1.00	35.40
60	ATOM	441	N	AARG	A	363	25.826	-10.059	-4.095	0.50	34.23
	ATOM	442	N	BARG	A	363	25.826	-10.059	-4.095	0.50	34.03

5	ATOM	443	CA	AARG	A	363	27.035	-9.254	-3.987	0.50	33.25
	ATOM	444	CA	BARG	A	363	27.035	-9.254	-3.987	0.50	32.83
	ATOM	445	CB	AARG	A	363	27.031	-8.153	-5.044	0.50	34.67
	ATOM	446	CB	BARG	A	363	27.031	-8.153	-5.045	0.50	34.20
	ATOM	447	CG	AARG	A	363	26.933	-8.654	-6.478	0.50	36.32
10	ATOM	448	CG	BARG	A	363	26.930	-8.654	-6.480	0.50	35.56
	ATOM	449	CD	AARG	A	363	27.745	-7.775	-7.415	0.50	38.39
	ATOM	450	CD	BARG	A	363	27.752	-7.781	-7.414	0.50	37.18
	ATOM	451	NE	AARG	A	363	29.171	-7.793	-7.091	0.50	39.98
	ATOM	452	NE	BARG	A	363	27.195	-7.725	-8.762	0.50	37.39
15	ATOM	453	CZ	AARG	A	363	30.086	-7.038	-7.692	0.50	40.54
	ATOM	454	CZ	BARG	A	363	27.905	-7.457	-9.855	0.50	40.02
	ATOM	455	NH1	AARG	A	363	29.735	-6.218	-8.675	0.50	38.13
	ATOM	456	NH1	BARG	A	363	29.205	-7.191	-9.761	0.50	40.42
	ATOM	457	NH2	AARG	A	363	31.358	-7.123	-7.326	0.50	43.19
20	ATOM	458	NH2	BARG	A	363	27.311	-7.436	-11.041	0.50	38.91
	ATOM	459	C	AARG	A	363	27.207	-8.630	-2.610	0.50	33.28
	ATOM	460	C	BARG	A	363	27.207	-8.630	-2.610	0.50	32.81
	ATOM	461	O	AARG	A	363	28.223	-7.992	-2.344	0.50	34.18
	ATOM	462	O	BARG	A	363	28.223	-7.992	-2.345	0.50	33.43
25	ATOM	463	N	VAL	A	364	26.215	-8.798	-1.740	1.00	33.12
	ATOM	464	CA	VAL	A	364	26.288	-8.240	-0.389	1.00	33.63
	ATOM	465	CB	VAL	A	364	24.898	-8.178	0.292	1.00	34.97
	ATOM	466	CG1	VAL	A	364	25.036	-7.608	1.700	1.00	35.44
	ATOM	467	CG2	VAL	A	364	23.946	-7.328	-0.532	1.00	36.69
30	ATOM	468	C	VAL	A	364	27.184	-9.157	0.428	1.00	34.27
	ATOM	469	O	VAL	A	364	26.878	-10.341	0.603	1.00	34.95
	ATOM	470	N	PRO	A	365	28.306	-8.626	0.935	1.00	36.08
	ATOM	471	CD	PRO	A	365	28.775	-7.235	0.793	1.00	34.84
	ATOM	472	CA	PRO	A	365	29.231	-9.442	1.733	1.00	37.82
35	ATOM	473	CB	PRO	A	365	30.110	-8.408	2.430	1.00	34.31
	ATOM	474	CG	PRO	A	365	30.127	-7.247	1.475	1.00	37.77
	ATOM	475	C	PRO	A	365	28.538	-10.373	2.720	1.00	37.61
	ATOM	476	O	PRO	A	365	27.692	-9.945	3.507	1.00	37.74
	ATOM	477	N	GLY	A	366	28.890	-11.654	2.654	1.00	39.04
40	ATOM	478	CA	GLY	A	366	28.307	-12.635	3.554	1.00	38.27
	ATOM	479	C	GLY	A	366	26.991	-13.264	3.138	1.00	39.32
	ATOM	480	O	GLY	A	366	26.638	-14.336	3.635	1.00	39.53
	ATOM	481	N	PHE	A	367	26.246	-12.615	2.236	1.00	38.60
	ATOM	482	CA	PHE	A	367	24.960	-13.148	1.783	1.00	36.36
45	ATOM	483	CB	PHE	A	367	24.281	-12.178	0.808	1.00	32.10
	ATOM	484	CG	PHE	A	367	22.827	-12.473	0.581	1.00	30.12
	ATOM	485	CD1	PHE	A	367	22.401	-13.083	-0.596	1.00	28.95
	ATOM	486	CD2	PHE	A	367	21.882	-12.176	1.563	1.00	26.18
	ATOM	487	CE1	PHE	A	367	21.050	-13.400	-0.792	1.00	29.42
50	ATOM	488	CE2	PHE	A	367	20.535	-12.491	1.373	1.00	27.60
	ATOM	489	CZ	PHE	A	367	20.118	-13.103	0.196	1.00	26.81
	ATOM	490	C	PHE	A	367	25.072	-14.519	1.117	1.00	36.82
	ATOM	491	O	PHE	A	367	24.244	-15.398	1.359	1.00	36.55
	ATOM	492	N	VAL	A	368	26.088	-14.694	0.276	1.00	38.28
55	ATOM	493	CA	VAL	A	368	26.289	-15.965	-0.420	1.00	42.34
	ATOM	494	CB	VAL	A	368	27.386	-15.850	-1.504	1.00	41.78
	ATOM	495	CG1	VAL	A	368	26.972	-14.831	-2.550	1.00	44.60
	ATOM	496	CG2	VAL	A	368	28.707	-15.457	-0.873	1.00	42.23
	ATOM	497	C	VAL	A	368	26.664	-17.100	0.533	1.00	43.85
60	ATOM	498	O	VAL	A	368	26.469	-18.274	0.216	1.00	44.85
	ATOM	499	N	ASP	A	369	27.199	-16.750	1.699	1.00	44.93

5	ATOM	500	CA	ASP	A	369	27.579	-17.755	2.688	1.00	44.96
	ATOM	501	CB	ASP	A	369	28.336	-17.106	3.849	1.00	43.76
	ATOM	502	CG	ASP	A	369	29.608	-16.413	3.404	1.00	43.04
	ATOM	503	OD1	ASP	A	369	30.121	-15.570	4.167	1.00	44.32
10	ATOM	504	OD2	ASP	A	369	30.097	-16.709	2.293	1.00	46.76
	ATOM	505	C	ASP	A	369	26.340	-18.465	3.228	1.00	45.89
	ATOM	506	O	ASP	A	369	26.360	-19.671	3.475	1.00	48.61
	ATOM	507	N	LEU	A	370	25.261	-17.714	3.407	1.00	43.59
15	ATOM	508	CA	LEU	A	370	24.020	-18.279	3.924	1.00	44.24
	ATOM	509	CB	LEU	A	370	22.980	-17.173	4.110	1.00	41.42
	ATOM	510	CG	LEU	A	370	23.404	-16.015	5.014	1.00	41.45
	ATOM	511	CD1	LEU	A	370	22.219	-15.095	5.245	1.00	42.25
20	ATOM	512	CD2	LEU	A	370	23.931	-16.552	6.332	1.00	38.35
	ATOM	513	C	LEU	A	370	23.449	-19.360	3.013	1.00	44.03
	ATOM	514	O	LEU	A	370	23.773	-19.423	1.829	1.00	43.63
	ATOM	515	N	THR	A	371	22.593	-20.206	3.575	1.00	44.29
25	ATOM	516	CA	THR	A	371	21.968	-21.272	2.806	1.00	44.84
	ATOM	517	CB	THR	A	371	21.293	-22.302	3.730	1.00	45.65
	ATOM	518	OG1	THR	A	371	20.262	-21.663	4.495	1.00	46.43
	ATOM	519	CG2	THR	A	371	22.314	-22.903	4.677	1.00	46.48
30	ATOM	520	C	THR	A	371	20.923	-20.684	1.864	1.00	44.93
	ATOM	521	O	THR	A	371	20.418	-19.585	2.092	1.00	44.36
	ATOM	522	N	LEU	A	372	20.607	-21.418	0.804	1.00	43.83
	ATOM	523	CA	LEU	A	372	19.624	-20.971	-0.166	1.00	44.62
35	ATOM	524	CB	LEU	A	372	19.407	-22.043	-1.237	1.00	47.17
	ATOM	525	CG	LEU	A	372	18.512	-21.690	-2.429	1.00	46.91
	ATOM	526	CD1	LEU	A	372	19.005	-20.417	-3.098	1.00	48.73
	ATOM	527	CD2	LEU	A	372	18.521	-22.844	-3.420	1.00	51.12
40	ATOM	528	C	LEU	A	372	18.307	-20.644	0.512	1.00	44.84
	ATOM	529	O	LEU	A	372	17.705	-19.602	0.261	1.00	43.25
	ATOM	530	N	HIS	A	373	17.849	-21.558	1.382	1.00	43.14
	ATOM	531	CA	HIS	A	373	16.599	-21.353	2.100	1.00	42.23
45	ATOM	532	CB	HIS	A	373	16.318	-22.525	3.062	1.00	45.38
	ATOM	533	CG	HIS	A	373	15.114	-22.315	3.934	1.00	51.43
	ATOM	534	CD2	HIS	A	373	13.808	-22.621	3.743	1.00	54.99
	ATOM	535	ND1	HIS	A	373	15.187	-21.716	5.174	1.00	54.26
50	ATOM	536	CE1	HIS	A	373	13.979	-21.663	5.709	1.00	53.77
	ATOM	537	NE2	HIS	A	373	13.124	-22.206	4.861	1.00	55.27
	ATOM	538	C	HIS	A	373	16.665	-20.047	2.885	1.00	39.78
	ATOM	539	O	HIS	A	373	15.677	-19.324	2.971	1.00	37.71
55	ATOM	540	N	ASP	A	374	17.839	-19.738	3.440	1.00	36.38
	ATOM	541	CA	ASP	A	374	18.020	-18.516	4.219	1.00	37.21
	ATOM	542	CB	ASP	A	374	19.287	-18.620	5.073	1.00	38.17
	ATOM	543	CG	ASP	A	374	19.064	-19.425	6.344	1.00	41.47
60	ATOM	544	OD1	ASP	A	374	17.896	-19.543	6.772	1.00	37.09
	ATOM	545	OD2	ASP	A	374	20.052	-19.940	6.912	1.00	44.40
	ATOM	546	C	ASP	A	374	18.083	-17.277	3.326	1.00	37.19
	ATOM	547	O	ASP	A	374	17.598	-16.208	3.696	1.00	38.13
55	ATOM	548	N	GLN	A	375	18.688	-17.431	2.152	1.00	33.13
	ATOM	549	CA	GLN	A	375	18.788	-16.339	1.198	1.00	31.94
	ATOM	550	CB	GLN	A	375	19.634	-16.756	-0.001	1.00	28.81
	ATOM	551	CG	GLN	A	375	21.125	-16.570	0.189	1.00	31.71
60	ATOM	552	CD	GLN	A	375	21.920	-17.222	-0.922	1.00	34.49
	ATOM	553	OE1	GLN	A	375	21.478	-17.267	-2.067	1.00	36.09
	ATOM	554	NE2	GLN	A	375	23.097	-17.736	-0.588	1.00	40.32
	ATOM	555	C	GLN	A	375	17.379	-16.009	0.730	1.00	31.50
	ATOM	556	O	GLN	A	375	16.990	-14.840	0.653	1.00	27.42

5	ATOM	557	N	VAL	A	376	16.617	-17.056	0.429	1.00	30.38
	ATOM	558	CA	VAL	A	376	15.242	-16.907	-0.027	1.00	33.50
	ATOM	559	CB	VAL	A	376	14.588	-18.286	-0.286	1.00	30.57
	ATOM	560	CG1	VAL	A	376	13.093	-18.122	-0.516	1.00	33.14
	ATOM	561	CG2	VAL	A	376	15.232	-18.952	-1.485	1.00	30.79
10	ATOM	562	C	VAL	A	376	14.393	-16.159	1.002	1.00	33.80
	ATOM	563	O	VAL	A	376	13.653	-15.237	0.661	1.00	34.89
	ATOM	564	N	HIS	A	377	14.500	-16.568	2.261	1.00	33.35
	ATOM	565	CA	HIS	A	377	13.730	-15.941	3.329	1.00	32.81
	ATOM	566	CB	HIS	A	377	13.966	-16.694	4.644	1.00	35.24
15	ATOM	567	CG	HIS	A	377	13.429	-15.989	5.851	1.00	40.15
	ATOM	568	CD2	HIS	A	377	14.054	-15.495	6.946	1.00	40.86
	ATOM	569	ND1	HIS	A	377	12.090	-15.703	6.012	1.00	43.08
	ATOM	570	CE1	HIS	A	377	11.913	-15.062	7.154	1.00	42.44
	ATOM	571	NE2	HIS	A	377	13.089	-14.922	7.740	1.00	44.85
20	ATOM	572	C	HIS	A	377	14.058	-14.454	3.507	1.00	28.63
	ATOM	573	O	HIS	A	377	13.158	-13.619	3.613	1.00	29.20
	ATOM	574	N	LEU	A	378	15.343	-14.125	3.544	1.00	24.41
	ATOM	575	CA	LEU	A	378	15.759	-12.738	3.721	1.00	23.21
	ATOM	576	CB	LEU	A	378	17.289	-12.650	3.743	1.00	20.98
25	ATOM	577	CG	LEU	A	378	17.960	-13.190	5.016	1.00	24.22
	ATOM	578	CD1	LEU	A	378	19.471	-13.041	4.924	1.00	21.07
	ATOM	579	CD2	LEU	A	378	17.431	-12.446	6.221	1.00	20.24
	ATOM	580	C	LEU	A	378	15.190	-11.827	2.630	1.00	24.78
	ATOM	581	O	LEU	A	378	14.638	-10.766	2.922	1.00	22.09
30	ATOM	582	N	LEU	A	379	15.321	-12.242	1.374	1.00	24.13
	ATOM	583	CA	LEU	A	379	14.812	-11.447	0.262	1.00	25.02
	ATOM	584	CB	LEU	A	379	15.307	-12.025	-1.062	1.00	27.12
	ATOM	585	CG	LEU	A	379	16.724	-11.600	-1.437	1.00	24.39
	ATOM	586	CD1	LEU	A	379	17.299	-12.557	-2.470	1.00	27.58
35	ATOM	587	CD2	LEU	A	379	16.679	-10.178	-1.983	1.00	29.05
	ATOM	588	C	LEU	A	379	13.287	-11.355	0.246	1.00	27.61
	ATOM	589	O	LEU	A	379	12.726	-10.301	-0.062	1.00	26.16
	ATOM	590	N	GLU	A	380	12.616	-12.454	0.576	1.00	25.65
	ATOM	591	CA	GLU	A	380	11.154	-12.471	0.592	1.00	26.85
40	ATOM	592	CB	GLU	A	380	10.640	-13.882	0.871	1.00	29.38
	ATOM	593	CG	GLU	A	380	10.718	-14.796	-0.331	1.00	35.58
	ATOM	594	CD	GLU	A	380	10.228	-16.194	-0.025	1.00	39.31
	ATOM	595	OE1	GLU	A	380	10.142	-17.008	-0.967	1.00	42.89
	ATOM	596	OE2	GLU	A	380	9.927	-16.478	1.153	1.00	39.45
45	ATOM	597	C	GLU	A	380	10.604	-11.526	1.649	1.00	25.43
	ATOM	598	O	GLU	A	380	9.551	-10.925	1.469	1.00	27.75
	ATOM	599	N	CYS	A	381	11.324	-11.400	2.753	1.00	25.57
	ATOM	600	CA	CYS	A	381	10.907	-10.530	3.843	1.00	26.46
	ATOM	601	CB	CYS	A	381	11.570	-11.000	5.149	1.00	31.46
50	ATOM	602	SG	CYS	A	381	11.305	-9.946	6.623	1.00	45.32
	ATOM	603	C	CYS	A	381	11.262	-9.059	3.589	1.00	24.77
	ATOM	604	O	CYS	A	381	10.516	-8.166	3.975	1.00	25.01
	ATOM	605	N	ALA	A	382	12.377	-8.815	2.903	1.00	22.23
	ATOM	606	CA	ALA	A	382	12.855	-7.449	2.681	1.00	21.83
55	ATOM	607	CB	ALA	A	382	14.319	-7.383	3.095	1.00	21.56
	ATOM	608	C	ALA	A	382	12.705	-6.778	1.311	1.00	19.78
	ATOM	609	O	ALA	A	382	12.996	-5.587	1.182	1.00	17.01
	ATOM	610	N	TRP	A	383	12.261	-7.507	0.294	1.00	17.61
	ATOM	611	CA	TRP	A	383	12.164	-6.915	-1.036	1.00	18.06
60	ATOM	612	CB	TRP	A	383	11.580	-7.928	-2.035	1.00	20.28
	ATOM	613	CG	TRP	A	383	10.105	-8.201	-1.919	1.00	20.50

5	ATOM	614	CD2	TRP	A	383	9.049	-7.509	-2.599	1.00	22.48
	ATOM	615	CE2	TRP	A	383	7.836	-8.138	-2.238	1.00	20.41
	ATOM	616	CE3	TRP	A	383	9.012	-6.420	-3.482	1.00	22.06
	ATOM	617	CD1	TRP	A	383	9.506	-9.189	-1.190	1.00	23.38
	ATOM	618	NE1	TRP	A	383	8.142	-9.159	-1.377	1.00	22.59
10	ATOM	619	CZ2	TRP	A	383	6.598	-7.713	-2.724	1.00	21.98
	ATOM	620	CZ3	TRP	A	383	7.780	-5.998	-3.968	1.00	25.50
	ATOM	621	CH2	TRP	A	383	6.589	-6.647	-3.587	1.00	23.11
	ATOM	622	C	TRP	A	383	11.448	-5.564	-1.170	1.00	19.18
	ATOM	623	O	TRP	A	383	11.972	-4.663	-1.824	1.00	19.27
15	ATOM	624	N	LEU	A	384	10.273	-5.396	-0.567	1.00	18.32
	ATOM	625	CA	LEU	A	384	9.586	-4.118	-0.719	1.00	16.38
	ATOM	626	CB	LEU	A	384	8.125	-4.218	-0.258	1.00	16.79
	ATOM	627	CG	LEU	A	384	7.211	-3.013	-0.577	1.00	18.39
	ATOM	628	CD1	LEU	A	384	7.464	-2.485	-1.995	1.00	13.91
20	ATOM	629	CD2	LEU	A	384	5.750	-3.432	-0.410	1.00	18.38
	ATOM	630	C	LEU	A	384	10.324	-3.027	0.051	1.00	18.80
	ATOM	631	O	LEU	A	384	10.334	-1.870	-0.357	1.00	20.90
	ATOM	632	N	GLU	A	385	10.949	-3.404	1.163	1.00	18.61
	ATOM	633	CA	GLU	A	385	11.718	-2.462	1.970	1.00	19.58
25	ATOM	634	CB	GLU	A	385	12.274	-3.154	3.213	1.00	17.43
	ATOM	635	CG	GLU	A	385	11.292	-3.237	4.357	1.00	22.92
	ATOM	636	CD	GLU	A	385	11.963	-3.676	5.640	1.00	25.83
	ATOM	637	OE1	GLU	A	385	12.431	-2.799	6.391	1.00	23.69
	ATOM	638	OE2	GLU	A	385	12.027	-4.897	5.889	1.00	27.64
30	ATOM	639	C	GLU	A	385	12.890	-1.934	1.156	1.00	19.46
	ATOM	640	O	GLU	A	385	13.206	-0.743	1.196	1.00	15.04
	ATOM	641	N	ILE	A	386	13.539	-2.842	0.431	1.00	13.32
	ATOM	642	CA	ILE	A	386	14.685	-2.484	-0.388	1.00	15.01
	ATOM	643	CB	ILE	A	386	15.475	-3.763	-0.807	1.00	17.43
35	ATOM	644	CG2	ILE	A	386	16.544	-3.424	-1.849	1.00	17.99
	ATOM	645	CG1	ILE	A	386	16.185	-4.338	0.432	1.00	20.31
	ATOM	646	CD1	ILE	A	386	16.682	-5.766	0.284	1.00	23.97
	ATOM	647	C	ILE	A	386	14.273	-1.645	-1.598	1.00	16.10
	ATOM	648	O	ILE	A	386	14.993	-0.724	-2.004	1.00	17.42
40	ATOM	649	N	LEU	A	387	13.112	-1.944	-2.167	1.00	17.61
	ATOM	650	CA	LEU	A	387	12.620	-1.173	-3.304	1.00	18.20
	ATOM	651	CB	LEU	A	387	11.359	-1.814	-3.882	1.00	17.51
	ATOM	652	CG	LEU	A	387	11.519	-3.064	-4.747	1.00	26.37
	ATOM	653	CD1	LEU	A	387	10.173	-3.406	-5.395	1.00	24.63
45	ATOM	654	CD2	LEU	A	387	12.589	-2.824	-5.808	1.00	21.58
	ATOM	655	C	LEU	A	387	12.283	0.249	-2.838	1.00	17.60
	ATOM	656	O	LEU	A	387	12.571	1.224	-3.530	1.00	17.15
	ATOM	657	N	MET	A	388	11.677	0.357	-1.660	1.00	17.65
	ATOM	658	CA	MET	A	388	11.286	1.656	-1.121	1.00	18.49
50	ATOM	659	CB	MET	A	388	10.302	1.460	0.034	1.00	19.65
	ATOM	660	CG	MET	A	388	8.893	1.105	-0.435	1.00	15.12
	ATOM	661	SD	MET	A	388	7.744	0.769	0.910	1.00	18.73
	ATOM	662	CE	MET	A	388	6.163	0.908	0.048	1.00	18.34
	ATOM	663	C	MET	A	388	12.451	2.553	-0.691	1.00	22.62
55	ATOM	664	O	MET	A	388	12.417	3.767	-0.928	1.00	22.49
	ATOM	665	N	ILE	A	389	13.482	1.988	-0.064	1.00	21.45
	ATOM	666	CA	ILE	A	389	14.604	2.831	0.331	1.00	18.54
	ATOM	667	CB	ILE	A	389	15.590	2.108	1.299	1.00	19.35
	ATOM	668	CG2	ILE	A	389	16.362	0.998	0.578	1.00	15.50
60	ATOM	669	CG1	ILE	A	389	16.556	3.142	1.889	1.00	21.95
	ATOM	670	CD1	ILE	A	389	17.373	2.658	3.080	1.00	15.86

5	ATOM	671	C	ILE	A	389	15.333	3.322	-0.922	1.00	18.67
	ATOM	672	O	ILE	A	389	15.813	4.453	-0.970	1.00	19.75
	ATOM	673	N	GLY	A	390	15.410	2.477	-1.943	1.00	20.58
	ATOM	674	CA	GLY	A	390	16.049	2.895	-3.183	1.00	19.33
	ATOM	675	C	GLY	A	390	15.243	4.021	-3.819	1.00	17.48
10	ATOM	676	O	GLY	A	390	15.801	4.994	-4.318	1.00	21.87
	ATOM	677	N	LEU	A	391	13.920	3.888	-3.787	1.00	19.17
	ATOM	678	CA	LEU	A	391	13.018	4.887	-4.343	1.00	21.50
	ATOM	679	CB	LEU	A	391	11.561	4.420	-4.194	1.00	18.25
	ATOM	680	CG	LEU	A	391	10.480	5.497	-4.342	1.00	21.98
15	ATOM	681	CD1	LEU	A	391	10.579	6.156	-5.725	1.00	21.39
	ATOM	682	CD2	LEU	A	391	9.115	4.868	-4.148	1.00	17.15
	ATOM	683	C	LEU	A	391	13.208	6.216	-3.620	1.00	23.27
	ATOM	684	O	LEU	A	391	13.440	7.255	-4.243	1.00	23.60
	ATOM	685	N	VAL	A	392	13.122	6.170	-2.295	1.00	23.04
20	ATOM	686	CA	VAL	A	392	13.282	7.357	-1.469	1.00	24.42
	ATOM	687	CB	VAL	A	392	13.186	6.993	0.042	1.00	27.38
	ATOM	688	CG1	VAL	A	392	13.733	8.129	0.897	1.00	30.37
	ATOM	689	CG2	VAL	A	392	11.739	6.712	0.414	1.00	23.48
	ATOM	690	C	VAL	A	392	14.626	8.014	-1.754	1.00	27.55
25	ATOM	691	O	VAL	A	392	14.728	9.242	-1.832	1.00	27.50
	ATOM	692	N	TRP	A	393	15.652	7.186	-1.924	1.00	23.65
	ATOM	693	CA	TRP	A	393	16.999	7.670	-2.204	1.00	24.76
	ATOM	694	CB	TRP	A	393	17.977	6.491	-2.199	1.00	22.86
	ATOM	695	CG	TRP	A	393	19.287	6.784	-2.857	1.00	25.90
30	ATOM	696	CD2	TRP	A	393	20.341	7.605	-2.339	1.00	28.09
	ATOM	697	CE2	TRP	A	393	21.375	7.612	-3.302	1.00	29.94
	ATOM	698	CE3	TRP	A	393	20.512	8.335	-1.154	1.00	30.20
	ATOM	699	CD1	TRP	A	393	19.710	6.339	-4.077	1.00	26.55
	ATOM	700	NE1	TRP	A	393	20.963	6.833	-4.351	1.00	30.64
35	ATOM	701	CZ2	TRP	A	393	22.566	8.323	-3.120	1.00	32.43
	ATOM	702	CZ3	TRP	A	393	21.698	9.044	-0.971	1.00	34.58
	ATOM	703	CH2	TRP	A	393	22.709	9.030	-1.950	1.00	36.54
	ATOM	704	C	TRP	A	393	17.082	8.414	-3.547	1.00	25.02
	ATOM	705	O	TRP	A	393	17.767	9.435	-3.650	1.00	20.97
40	ATOM	706	N	ARG	A	394	16.399	7.897	-4.568	1.00	23.06
	ATOM	707	CA	ARG	A	394	16.412	8.531	-5.890	1.00	25.97
	ATOM	708	CB	ARG	A	394	15.776	7.633	-6.965	1.00	24.05
	ATOM	709	CG	ARG	A	394	16.243	6.195	-7.024	1.00	26.05
	ATOM	710	CD	ARG	A	394	15.830	5.551	-8.352	1.00	22.70
45	ATOM	711	NE	ARG	A	394	14.443	5.071	-8.363	1.00	20.71
	ATOM	712	CZ	ARG	A	394	14.053	3.912	-7.841	1.00	21.26
	ATOM	713	NH1	ARG	A	394	14.944	3.108	-7.267	1.00	20.09
	ATOM	714	NH2	ARG	A	394	12.783	3.544	-7.907	1.00	21.26
	ATOM	715	C	ARG	A	394	15.622	9.833	-5.879	1.00	23.40
50	ATOM	716	O	ARG	A	394	15.889	10.729	-6.677	1.00	28.61
	ATOM	717	N	SER	A	395	14.638	9.924	-4.988	1.00	26.65
	ATOM	718	CA	SER	A	395	13.776	11.104	-4.902	1.00	27.46
	ATOM	719	CB	SER	A	395	12.395	10.696	-4.382	1.00	26.70
	ATOM	720	OG	SER	A	395	11.916	9.530	-5.029	1.00	22.95
55	ATOM	721	C	SER	A	395	14.316	12.240	-4.033	1.00	31.45
	ATOM	722	O	SER	A	395	13.726	13.324	-3.977	1.00	28.11
	ATOM	723	N	MET	A	396	15.437	11.986	-3.368	1.00	33.83
	ATOM	724	CA	MET	A	396	16.061	12.954	-2.475	1.00	38.83
	ATOM	725	CB	MET	A	396	17.466	12.483	-2.112	1.00	39.47
60	ATOM	726	CG	MET	A	396	17.585	11.919	-0.715	1.00	41.37
	ATOM	727	SD	MET	A	396	19.192	12.262	0.004	1.00	42.20

5	ATOM	728	CE	MET	A	396	20.263	11.996	-1.404	1.00	42.84
	ATOM	729	C	MET	A	396	16.143	14.376	-3.018	1.00	40.69
	ATOM	730	O	MET	A	396	15.637	15.316	-2.403	1.00	38.85
	ATOM	731	N	GLU	A	397	16.794	14.526	-4.166	1.00	42.19
	ATOM	732	CA	GLU	A	397	16.971	15.831	-4.790	1.00	44.80
10	ATOM	733	CB	GLU	A	397	18.184	15.785	-5.729	1.00	46.02
	ATOM	734	CG	GLU	A	397	17.883	15.189	-7.096	1.00	54.42
	ATOM	735	CD	GLU	A	397	19.117	14.665	-7.810	1.00	59.40
	ATOM	736	OE1	GLU	A	397	19.219	13.430	-7.990	1.00	60.63
	ATOM	737	OE2	GLU	A	397	19.980	15.485	-8.196	1.00	62.71
15	ATOM	738	C	GLU	A	397	15.735	16.322	-5.554	1.00	42.94
	ATOM	739	O	GLU	A	397	15.830	17.229	-6.376	1.00	44.68
	ATOM	740	N	HIS	A	398	14.579	15.728	-5.280	1.00	40.82
	ATOM	741	CA	HIS	A	398	13.342	16.118	-5.950	1.00	39.21
	ATOM	742	CB	HIS	A	398	12.924	15.043	-6.956	1.00	39.05
20	ATOM	743	CG	HIS	A	398	13.870	14.886	-8.104	1.00	41.57
	ATOM	744	CD2	HIS	A	398	13.904	15.484	-9.318	1.00	39.28
	ATOM	745	ND1	HIS	A	398	14.940	14.017	-8.074	1.00	41.85
	ATOM	746	CE1	HIS	A	398	15.592	14.086	-9.220	1.00	40.88
	ATOM	747	NE2	HIS	A	398	14.985	14.969	-9.993	1.00	42.30
25	ATOM	748	C	HIS	A	398	12.216	16.332	-4.944	1.00	37.04
	ATOM	749	O	HIS	A	398	11.282	15.535	-4.864	1.00	36.51
	ATOM	750	N	PRO	A	399	12.283	17.427	-4.171	1.00	39.19
	ATOM	751	CD	PRO	A	399	13.328	18.467	-4.198	1.00	35.36
	ATOM	752	CA	PRO	A	399	11.243	17.709	-3.173	1.00	37.10
30	ATOM	753	CB	PRO	A	399	11.603	19.101	-2.654	1.00	37.86
	ATOM	754	CG	PRO	A	399	13.050	19.267	-2.963	1.00	35.83
	ATOM	755	C	PRO	A	399	9.828	17.663	-3.744	1.00	37.02
	ATOM	756	O	PRO	A	399	9.554	18.249	-4.789	1.00	38.52
	ATOM	757	N	GLY	A	400	8.938	16.954	-3.057	1.00	33.58
35	ATOM	758	CA	GLY	A	400	7.559	16.865	-3.503	1.00	32.12
	ATOM	759	C	GLY	A	400	7.230	15.706	-4.428	1.00	32.43
	ATOM	760	O	GLY	A	400	6.063	15.344	-4.574	1.00	33.21
	ATOM	761	N	LYS	A	401	8.237	15.112	-5.055	1.00	31.35
	ATOM	762	CA	LYS	A	401	7.972	14.007	-5.966	1.00	30.75
40	ATOM	763	CB	LYS	A	401	8.235	14.430	-7.415	1.00	35.43
	ATOM	764	CG	LYS	A	401	8.130	15.927	-7.675	1.00	35.15
	ATOM	765	CD	LYS	A	401	9.096	16.353	-8.774	1.00	36.88
	ATOM	766	CE	LYS	A	401	8.733	17.721	-9.331	1.00	36.71
	ATOM	767	NZ	LYS	A	401	7.295	18.027	-9.116	1.00	34.22
45	ATOM	768	C	LYS	A	401	8.768	12.746	-5.677	1.00	30.97
	ATOM	769	O	LYS	A	401	9.809	12.776	-5.006	1.00	27.60
	ATOM	770	N	LEU	A	402	8.256	11.635	-6.197	1.00	27.28
	ATOM	771	CA	LEU	A	402	8.889	10.334	-6.050	1.00	29.07
	ATOM	772	CB	LEU	A	402	7.866	9.294	-5.590	1.00	22.55
50	ATOM	773	CG	LEU	A	402	7.265	9.555	-4.207	1.00	24.94
	ATOM	774	CD1	LEU	A	402	6.126	8.583	-3.937	1.00	19.32
	ATOM	775	CD2	LEU	A	402	8.355	9.416	-3.157	1.00	21.54
	ATOM	776	C	LEU	A	402	9.448	9.948	-7.414	1.00	28.78
	ATOM	777	O	LEU	A	402	8.704	9.836	-8.389	1.00	29.98
55	ATOM	778	N	LEU	A	403	10.761	9.770	-7.487	1.00	27.57
	ATOM	779	CA	LEU	A	403	11.393	9.400	-8.744	1.00	27.17
	ATOM	780	CB	LEU	A	403	12.825	9.937	-8.816	1.00	26.95
	ATOM	781	CG	LEU	A	403	13.401	10.027	-10.238	1.00	30.42
	ATOM	782	CD1	LEU	A	403	14.519	11.046	-10.288	1.00	30.76
60	ATOM	783	CD2	LEU	A	403	13.915	8.665	-10.676	1.00	33.11
	ATOM	784	C	LEU	A	403	11.419	7.891	-8.901	1.00	24.78



5	ATOM	785	O	LEU	A	403	12.428	7.257	-8.619	1.00	24.68
	ATOM	786	N	PHE	A	404	10.306	7.319	-9.344	1.00	23.11
	ATOM	787	CA	PHE	A	404	10.239	5.881	-9.546	1.00	26.93
	ATOM	788	CB	PHE	A	404	8.826	5.470	-9.946	1.00	27.04
	ATOM	789	CG	PHE	A	404	7.850	5.513	-8.816	1.00	27.89
10	ATOM	790	CD1	PHE	A	404	7.028	6.623	-8.631	1.00	26.20
	ATOM	791	CD2	PHE	A	404	7.750	4.444	-7.925	1.00	23.10
	ATOM	792	CE1	PHE	A	404	6.116	6.668	-7.573	1.00	25.29
	ATOM	793	CE2	PHE	A	404	6.845	4.481	-6.870	1.00	21.01
	ATOM	794	CZ	PHE	A	404	6.026	5.595	-6.693	1.00	22.91
15	ATOM	795	C	PHE	A	404	11.232	5.507	-10.637	1.00	26.04
	ATOM	796	O	PHE	A	404	11.882	4.464	-10.578	1.00	27.27
	ATOM	797	N	ALA	A	405	11.348	6.383	-11.626	1.00	28.80
	ATOM	798	CA	ALA	A	405	12.271	6.195	-12.740	1.00	29.21
	ATOM	799	CB	ALA	A	405	11.650	5.287	-13.806	1.00	26.89
20	ATOM	800	C	ALA	A	405	12.549	7.578	-13.317	1.00	30.23
	ATOM	801	O	ALA	A	405	11.770	8.508	-13.109	1.00	27.38
	ATOM	802	N	PRO	A	406	13.672	7.737	-14.032	1.00	30.05
	ATOM	803	CD	PRO	A	406	14.712	6.745	-14.352	1.00	26.31
	ATOM	804	CA	PRO	A	406	13.977	9.053	-14.604	1.00	32.10
25	ATOM	805	CB	PRO	A	406	15.232	8.800	-15.438	1.00	31.28
	ATOM	806	CG	PRO	A	406	15.865	7.602	-14.776	1.00	31.44
	ATOM	807	C	PRO	A	406	12.820	9.589	-15.436	1.00	32.58
	ATOM	808	O	PRO	A	406	12.605	10.796	-15.507	1.00	32.58
	ATOM	809	N	ASN	A	407	12.063	8.690	-16.053	1.00	32.86
30	ATOM	810	CA	ASN	A	407	10.935	9.119	-16.865	1.00	32.78
	ATOM	811	CB	ASN	A	407	10.950	8.418	-18.228	1.00	34.73
	ATOM	812	CG	ASN	A	407	10.884	6.907	-18.121	1.00	35.37
	ATOM	813	OD1	ASN	A	407	11.189	6.317	-17.077	1.00	30.24
	ATOM	814	ND2	ASN	A	407	10.486	6.268	-19.215	1.00	34.08
35	ATOM	815	C	ASN	A	407	9.605	8.901	-16.166	1.00	34.90
	ATOM	816	O	ASN	A	407	8.549	8.897	-16.798	1.00	36.09
	ATOM	817	N	LEU	A	408	9.660	8.724	-14.851	1.00	33.56
	ATOM	818	CA	LEU	A	408	8.452	8.544	-14.061	1.00	35.59
	ATOM	819	CB	LEU	A	408	8.141	7.062	-13.851	1.00	33.81
40	ATOM	820	CG	LEU	A	408	6.696	6.823	-13.397	1.00	36.44
	ATOM	821	CD1	LEU	A	408	5.746	7.479	-14.390	1.00	34.14
	ATOM	822	CD2	LEU	A	408	6.406	5.334	-13.287	1.00	32.96
	ATOM	823	C	LEU	A	408	8.607	9.245	-12.717	1.00	38.03
	ATOM	824	O	LEU	A	408	8.880	8.614	-11.695	1.00	36.38
45	ATOM	825	N	LEU	A	409	8.441	10.563	-12.741	1.00	37.87
	ATOM	826	CA	LEU	A	409	8.548	11.395	-11.553	1.00	37.95
	ATOM	827	CB	LEU	A	409	9.373	12.636	-11.877	1.00	39.52
	ATOM	828	CG	LEU	A	409	10.023	13.399	-10.728	1.00	42.46
	ATOM	829	CD1	LEU	A	409	11.100	12.547	-10.082	1.00	43.24
50	ATOM	830	CD2	LEU	A	409	10.614	14.691	-11.266	1.00	46.05
	ATOM	831	C	LEU	A	409	7.132	11.792	-11.163	1.00	37.13
	ATOM	832	O	LEU	A	409	6.482	12.546	-11.882	1.00	35.70
	ATOM	833	N	LEU	A	410	6.654	11.284	-10.030	1.00	35.29
	ATOM	834	CA	LEU	A	410	5.297	11.576	-9.583	1.00	33.33
55	ATOM	835	CB	LEU	A	410	4.503	10.277	-9.449	1.00	29.37
	ATOM	836	CG	LEU	A	410	4.645	9.238	-10.560	1.00	32.75
	ATOM	837	CD1	LEU	A	410	4.026	7.925	-10.104	1.00	29.16
	ATOM	838	CD2	LEU	A	410	3.958	9.744	-11.819	1.00	30.70
	ATOM	839	C	LEU	A	410	5.207	12.332	-8.261	1.00	35.14
60	ATOM	840	O	LEU	A	410	6.078	12.214	-7.400	1.00	36.94
	ATOM	841	N	ASP	A	411	4.141	13.108	-8.105	1.00	34.76

5	ATOM	842	CA	ASP	A	411	3.933	13.843	-6.873	1.00	35.40
	ATOM	843	CB	ASP	A	411	3.733	15.341	-7.144	1.00	40.02
	ATOM	844	CG	ASP	A	411	2.471	15.645	-7.928	1.00	41.32
	ATOM	845	OD1	ASP	A	411	1.570	14.785	-8.001	1.00	45.03
10	ATOM	846	OD2	ASP	A	411	2.383	16.764	-8.474	1.00	45.01
	ATOM	847	C	ASP	A	411	2.727	13.234	-6.179	1.00	36.10
	ATOM	848	O	ASP	A	411	2.033	12.395	-6.762	1.00	34.08
	ATOM	849	N	ARG	A	412	2.480	13.647	-4.940	1.00	35.99
15	ATOM	850	CA	ARG	A	412	1.375	13.099	-4.169	1.00	39.37
	ATOM	851	CB	ARG	A	412	1.260	13.824	-2.825	1.00	39.75
	ATOM	852	CG	ARG	A	412	0.562	15.168	-2.870	1.00	40.49
	ATOM	853	CD	ARG	A	412	0.454	15.736	-1.465	1.00	40.65
20	ATOM	854	NE	ARG	A	412	-0.261	14.826	-0.577	1.00	37.48
	ATOM	855	CZ	ARG	A	412	-1.574	14.855	-0.384	1.00	42.84
	ATOM	856	NH1	ARG	A	412	-2.316	15.754	-1.024	1.00	40.82
	ATOM	857	NH2	ARG	A	412	-2.150	13.986	0.438	1.00	38.32
25	ATOM	858	C	ARG	A	412	0.034	13.108	-4.889	1.00	39.80
	ATOM	859	O	ARG	A	412	-0.775	12.201	-4.706	1.00	39.92
	ATOM	860	N	ASN	A	413	-0.198	14.119	-5.717	1.00	41.64
	ATOM	861	CA	ASN	A	413	-1.458	14.215	-6.440	1.00	43.19
30	ATOM	862	CB	ASN	A	413	-1.518	15.533	-7.210	1.00	46.44
	ATOM	863	CG	ASN	A	413	-1.739	16.718	-6.299	1.00	47.86
	ATOM	864	OD1	ASN	A	413	-2.376	16.594	-5.249	1.00	48.05
	ATOM	865	ND2	ASN	A	413	-1.213	17.876	-6.687	1.00	49.43
35	ATOM	866	C	ASN	A	413	-1.673	13.044	-7.385	1.00	41.48
	ATOM	867	O	ASN	A	413	-2.792	12.567	-7.546	1.00	40.50
	ATOM	868	N	GLN	A	414	-0.600	12.577	-8.010	1.00	42.82
	ATOM	869	CA	GLN	A	414	-0.703	11.448	-8.925	1.00	44.73
40	ATOM	870	CB	GLN	A	414	0.585	11.307	-9.741	1.00	47.52
	ATOM	871	CG	GLN	A	414	0.572	12.088	-11.049	1.00	50.47
	ATOM	872	CD	GLN	A	414	1.914	12.713	-11.375	1.00	53.91
	ATOM	873	OE1	GLN	A	414	2.591	13.257	-10.501	1.00	53.68
45	ATOM	874	NE2	GLN	A	414	2.309	12.637	-12.641	1.00	56.91
	ATOM	875	C	GLN	A	414	-0.970	10.163	-8.141	1.00	43.21
	ATOM	876	O	GLN	A	414	-1.491	9.193	-8.682	1.00	42.33
	ATOM	877	N	GLY	A	415	-0.618	10.168	-6.860	1.00	41.97
50	ATOM	878	CA	GLY	A	415	-0.836	8.992	-6.040	1.00	40.43
	ATOM	879	C	GLY	A	415	-2.306	8.720	-5.804	1.00	40.80
	ATOM	880	O	GLY	A	415	-2.696	7.601	-5.472	1.00	37.83
	ATOM	881	N	LYS	A	416	-3.129	9.748	-5.978	1.00	42.16
55	ATOM	882	CA	LYS	A	416	-4.566	9.613	-5.779	1.00	44.34
	ATOM	883	CB	LYS	A	416	-5.212	10.996	-5.704	1.00	45.65
	ATOM	884	CG	LYS	A	416	-4.761	11.819	-4.510	1.00	47.42
	ATOM	885	CD	LYS	A	416	-4.910	13.309	-4.777	1.00	50.97
60	ATOM	886	CE	LYS	A	416	-5.992	13.924	-3.898	1.00	53.25
	ATOM	887	NZ	LYS	A	416	-5.416	14.764	-2.809	1.00	56.95
	ATOM	888	C	LYS	A	416	-5.227	8.793	-6.886	1.00	45.33
	ATOM	889	O	LYS	A	416	-6.339	8.299	-6.714	1.00	46.50
65	ATOM	890	N	CYS	A	417	-4.540	8.648	-8.015	1.00	45.18
	ATOM	891	CA	CYS	A	417	-5.066	7.890	-9.148	1.00	46.25
	ATOM	892	CB	CYS	A	417	-4.062	7.902	-10.305	1.00	49.29
	ATOM	893	SG	CYS	A	417	-3.916	9.493	-11.168	1.00	49.59
70	ATOM	894	C	CYS	A	417	-5.373	6.452	-8.752	1.00	47.18
	ATOM	895	O	CYS	A	417	-6.220	5.794	-9.359	1.00	46.50
	ATOM	896	N	VAL	A	418	-4.671	5.968	-7.731	1.00	45.07
	ATOM	897	CA	VAL	A	418	-4.866	4.612	-7.232	1.00	42.75
75	ATOM	898	CB	VAL	A	418	-3.525	3.841	-7.206	1.00	42.45

5	ATOM	899	CG1	VAL	A	418	-3.670	2.563	-6.410	1.00	40.22
	ATOM	900	CG2	VAL	A	418	-3.071	3.538	-8.634	1.00	38.03
	ATOM	901	C	VAL	A	418	-5.441	4.714	-5.818	1.00	41.46
	ATOM	902	O	VAL	A	418	-4.883	5.400	-4.963	1.00	42.08
	ATOM	903	N	GLU	A	419	-6.559	4.036	-5.579	1.00	40.95
10	ATOM	904	CA	GLU	A	419	-7.223	4.073	-4.275	1.00	42.51
	ATOM	905	CB	GLU	A	419	-8.536	3.282	-4.333	1.00	44.52
	ATOM	906	CG	GLU	A	419	-9.010	2.751	-2.984	1.00	50.42
	ATOM	907	CD	GLU	A	419	-10.413	2.168	-3.035	1.00	54.38
	ATOM	908	OE1	GLU	A	419	-10.582	1.059	-3.590	1.00	54.09
15	ATOM	909	OE2	GLU	A	419	-11.347	2.820	-2.516	1.00	57.90
	ATOM	910	C	GLU	A	419	-6.370	3.552	-3.121	1.00	41.11
	ATOM	911	O	GLU	A	419	-5.955	2.393	-3.116	1.00	39.42
	ATOM	912	N	GLY	A	420	-6.129	4.419	-2.140	1.00	40.53
	ATOM	913	CA	GLY	A	420	-5.346	4.049	-0.973	1.00	37.61
20	ATOM	914	C	GLY	A	420	-3.854	4.258	-1.140	1.00	37.01
	ATOM	915	O	GLY	A	420	-3.088	4.105	-0.190	1.00	32.59
	ATOM	916	N	MET	A	421	-3.444	4.623	-2.350	1.00	36.21
	ATOM	917	CA	MET	A	421	-2.035	4.825	-2.656	1.00	36.02
	ATOM	918	CB	MET	A	421	-1.799	4.607	-4.160	1.00	32.84
25	ATOM	919	CG	MET	A	421	-0.351	4.754	-4.617	1.00	35.82
	ATOM	920	SD	MET	A	421	0.806	3.611	-3.812	1.00	35.57
	ATOM	921	CE	MET	A	421	0.881	2.294	-5.005	1.00	32.51
	ATOM	922	C	MET	A	421	-1.474	6.180	-2.226	1.00	34.93
	ATOM	923	O	MET	A	421	-0.275	6.294	-1.985	1.00	35.17
30	ATOM	924	N	VAL	A	422	-2.319	7.205	-2.118	1.00	33.97
	ATOM	925	CA	VAL	A	422	-1.823	8.520	-1.708	1.00	31.29
	ATOM	926	CB	VAL	A	422	-2.927	9.607	-1.766	1.00	33.14
	ATOM	927	CG1	VAL	A	422	-3.823	9.535	-0.533	1.00	30.10
	ATOM	928	CG2	VAL	A	422	-2.279	10.982	-1.854	1.00	30.08
35	ATOM	929	C	VAL	A	422	-1.231	8.498	-0.296	1.00	32.64
	ATOM	930	O	VAL	A	422	-0.274	9.220	0.002	1.00	28.41
	ATOM	931	N	GLU	A	423	-1.803	7.670	0.571	1.00	31.53
	ATOM	932	CA	GLU	A	423	-1.311	7.558	1.935	1.00	35.99
	ATOM	933	CB	GLU	A	423	-2.190	6.594	2.737	1.00	40.37
40	ATOM	934	CG	GLU	A	423	-3.588	7.129	3.043	1.00	49.41
	ATOM	935	CD	GLU	A	423	-4.438	7.336	1.795	1.00	52.38
	ATOM	936	OE1	GLU	A	423	-5.349	8.188	1.835	1.00	56.91
	ATOM	937	OE2	GLU	A	423	-4.200	6.652	0.776	1.00	54.53
	ATOM	938	C	GLU	A	423	0.127	7.043	1.886	1.00	34.83
45	ATOM	939	O	GLU	A	423	1.007	7.552	2.581	1.00	31.85
	ATOM	940	N	ILE	A	424	0.369	6.038	1.050	1.00	30.17
	ATOM	941	CA	ILE	A	424	1.711	5.488	0.929	1.00	28.99
	ATOM	942	CB	ILE	A	424	1.696	4.195	0.109	1.00	30.96
	ATOM	943	CG2	ILE	A	424	3.108	3.588	0.068	1.00	27.20
50	ATOM	944	CG1	ILE	A	424	0.671	3.230	0.725	1.00	30.77
	ATOM	945	CD1	ILE	A	424	0.810	1.787	0.291	1.00	34.69
	ATOM	946	C	ILE	A	424	2.700	6.483	0.312	1.00	28.21
	ATOM	947	O	ILE	A	424	3.856	6.551	0.735	1.00	28.48
	ATOM	948	N	PHE	A	425	2.253	7.260	-0.675	1.00	27.68
55	ATOM	949	CA	PHE	A	425	3.119	8.253	-1.315	1.00	27.30
	ATOM	950	CB	PHE	A	425	2.381	8.958	-2.458	1.00	26.36
	ATOM	951	CG	PHE	A	425	2.538	8.289	-3.798	1.00	27.22
	ATOM	952	CD1	PHE	A	425	2.619	9.050	-4.958	1.00	27.36
	ATOM	953	CD2	PHE	A	425	2.566	6.900	-3.905	1.00	27.89
60	ATOM	954	CE1	PHE	A	425	2.721	8.443	-6.207	1.00	29.63
	ATOM	955	CE2	PHE	A	425	2.668	6.282	-5.149	1.00	27.28

5	ATOM	956	CZ	PHE	A	425	2.745	7.056	-6.303	1.00	27.63
	ATOM	957	C	PHE	A	425	3.591	9.306	-0.312	1.00	25.66
	ATOM	958	O	PHE	A	425	4.757	9.713	-0.328	1.00	26.33
	ATOM	959	N	ASP	A	426	2.680	9.746	0.552	1.00	27.92
10	ATOM	960	CA	ASP	A	426	2.984	10.759	1.570	1.00	28.88
	ATOM	961	CB	ASP	A	426	1.721	11.102	2.369	1.00	32.58
	ATOM	962	CG	ASP	A	426	0.781	12.034	1.613	1.00	37.47
	ATOM	963	OD1	ASP	A	426	-0.432	12.039	1.925	1.00	37.72
15	ATOM	964	OD2	ASP	A	426	1.253	12.758	0.710	1.00	36.35
	ATOM	965	C	ASP	A	426	4.071	10.278	2.532	1.00	26.96
	ATOM	966	O	ASP	A	426	4.974	11.030	2.900	1.00	27.20
	ATOM	967	N	MET	A	427	3.978	9.022	2.947	1.00	25.76
20	ATOM	968	CA	MET	A	427	4.981	8.468	3.856	1.00	25.89
	ATOM	969	CB	MET	A	427	4.567	7.070	4.309	1.00	21.17
	ATOM	970	CG	MET	A	427	3.385	7.072	5.257	1.00	24.38
	ATOM	971	SD	MET	A	427	3.153	5.489	6.080	1.00	34.32
25	ATOM	972	CE	MET	A	427	2.173	4.637	4.910	1.00	21.03
	ATOM	973	C	MET	A	427	6.321	8.410	3.128	1.00	22.29
	ATOM	974	O	MET	A	427	7.363	8.760	3.689	1.00	22.19
	ATOM	975	N	LEU	A	428	6.285	7.985	1.868	1.00	21.75
30	ATOM	976	CA	LEU	A	428	7.506	7.892	1.075	1.00	22.91
	ATOM	977	CB	LEU	A	428	7.202	7.252	-0.287	1.00	18.47
	ATOM	978	CG	LEU	A	428	6.910	5.747	-0.176	1.00	19.24
	ATOM	979	CD1	LEU	A	428	6.278	5.222	-1.468	1.00	16.82
35	ATOM	980	CD2	LEU	A	428	8.204	5.010	0.131	1.00	16.23
	ATOM	981	C	LEU	A	428	8.148	9.269	0.902	1.00	23.98
	ATOM	982	O	LEU	A	428	9.366	9.416	1.034	1.00	23.06
	ATOM	983	N	LEU	A	429	7.328	10.281	0.628	1.00	23.91
40	ATOM	984	CA	LEU	A	429	7.837	11.642	0.462	1.00	26.29
	ATOM	985	CB	LEU	A	429	6.714	12.571	-0.003	1.00	27.47
	ATOM	986	CG	LEU	A	429	6.331	12.411	-1.476	1.00	30.78
	ATOM	987	CD1	LEU	A	429	5.022	13.139	-1.751	1.00	34.75
45	ATOM	988	CD2	LEU	A	429	7.449	12.952	-2.350	1.00	31.96
	ATOM	989	C	LEU	A	429	8.425	12.166	1.776	1.00	25.83
	ATOM	990	O	LEU	A	429	9.482	12.808	1.793	1.00	26.42
	ATOM	991	N	ALA	A	430	7.734	11.890	2.877	1.00	26.45
50	ATOM	992	CA	ALA	A	430	8.201	12.333	4.185	1.00	26.11
	ATOM	993	CB	ALA	A	430	7.214	11.909	5.265	1.00	23.13
	ATOM	994	C	ALA	A	430	9.577	11.742	4.462	1.00	25.01
	ATOM	995	O	ALA	A	430	10.455	12.409	5.005	1.00	24.31
55	ATOM	996	N	THR	A	431	9.767	10.486	4.074	1.00	25.25
	ATOM	997	CA	THR	A	431	11.046	9.825	4.294	1.00	22.78
	ATOM	998	CB	THR	A	431	10.973	8.323	3.962	1.00	21.36
	ATOM	999	OG1	THR	A	431	9.924	7.727	4.727	1.00	20.27
60	ATOM	1000	CG2	THR	A	431	12.291	7.633	4.299	1.00	19.99
	ATOM	1001	C	THR	A	431	12.103	10.477	3.429	1.00	23.73
	ATOM	1002	O	THR	A	431	13.234	10.667	3.868	1.00	19.60
	ATOM	1003	N	SER	A	432	11.736	10.819	2.197	1.00	24.32
55	ATOM	1004	CA	SER	A	432	12.676	11.479	1.301	1.00	26.96
	ATOM	1005	CB	SER	A	432	12.067	11.650	-0.093	1.00	28.70
	ATOM	1006	OG	SER	A	432	13.084	11.930	-1.039	1.00	33.42
	ATOM	1007	C	SER	A	432	13.033	12.850	1.876	1.00	27.92
60	ATOM	1008	O	SER	A	432	14.176	13.294	1.779	1.00	30.78
	ATOM	1009	N	SER	A	433	12.045	13.521	2.459	1.00	28.96
	ATOM	1010	CA	SER	A	433	12.269	14.824	3.076	1.00	34.21
	ATOM	1011	CB	SER	A	433	10.957	15.387	3.623	1.00	35.07
	ATOM	1012	OG	SER	A	433	10.175	15.961	2.591	1.00	42.38

5	ATOM	1013	C	SER	A	433	13.263	14.644	4.223	1.00	33.43
	ATOM	1014	O	SER	A	433	14.152	15.473	4.429	1.00	31.94
	ATOM	1015	N	ARG	A	434	13.105	13.545	4.959	1.00	31.32
	ATOM	1016	CA	ARG	A	434	13.980	13.236	6.086	1.00	29.78
	ATOM	1017	CB	ARG	A	434	13.468	11.994	6.819	1.00	29.84
10	ATOM	1018	CG	ARG	A	434	14.331	11.541	7.983	1.00	32.17
	ATOM	1019	CD	ARG	A	434	14.626	12.672	8.958	1.00	37.00
	ATOM	1020	NE	ARG	A	434	15.321	12.169	10.140	1.00	39.44
	ATOM	1021	CZ	ARG	A	434	15.935	12.935	11.034	1.00	44.06
	ATOM	1022	NH1	ARG	A	434	15.949	14.255	10.885	1.00	45.52
15	ATOM	1023	NH2	ARG	A	434	16.528	12.381	12.084	1.00	45.01
	ATOM	1024	C	ARG	A	434	15.413	13.014	5.605	1.00	29.24
	ATOM	1025	O	ARG	A	434	16.352	13.563	6.173	1.00	29.72
	ATOM	1026	N	PHE	A	435	15.577	12.206	4.561	1.00	28.95
	ATOM	1027	CA	PHE	A	435	16.901	11.935	4.000	1.00	30.59
20	ATOM	1028	CB	PHE	A	435	16.777	11.045	2.758	1.00	32.03
	ATOM	1029	CG	PHE	A	435	16.795	9.563	3.051	1.00	31.88
	ATOM	1030	CD1	PHE	A	435	16.758	9.084	4.359	1.00	35.60
	ATOM	1031	CD2	PHE	A	435	16.847	8.643	2.009	1.00	35.89
	ATOM	1032	CE1	PHE	A	435	16.771	7.709	4.622	1.00	35.36
25	ATOM	1033	CE2	PHE	A	435	16.860	7.271	2.262	1.00	32.71
	ATOM	1034	CZ	PHE	A	435	16.821	6.807	3.570	1.00	33.24
	ATOM	1035	C	PHE	A	435	17.576	13.253	3.607	1.00	32.73
	ATOM	1036	O	PHE	A	435	18.763	13.464	3.871	1.00	31.16
	ATOM	1037	N	ARG	A	436	16.812	14.137	2.975	1.00	33.37
30	ATOM	1038	CA	ARG	A	436	17.341	15.429	2.549	1.00	39.13
	ATOM	1039	CB	ARG	A	436	16.282	16.206	1.756	1.00	40.42
	ATOM	1040	CG	ARG	A	436	16.846	17.317	0.877	1.00	43.09
	ATOM	1041	CD	ARG	A	436	15.750	17.960	0.040	1.00	44.53
	ATOM	1042	NE	ARG	A	436	14.826	16.955	-0.472	1.00	48.34
35	ATOM	1043	CZ	ARG	A	436	13.530	16.913	-0.184	1.00	48.81
	ATOM	1044	NH1	ARG	A	436	12.997	17.823	0.619	1.00	47.80
	ATOM	1045	NH2	ARG	A	436	12.769	15.950	-0.687	1.00	49.53
	ATOM	1046	C	ARG	A	436	17.792	16.250	3.753	1.00	38.10
	ATOM	1047	O	ARG	A	436	18.896	16.789	3.764	1.00	41.00
40	ATOM	1048	N	MET	A	437	16.936	16.334	4.766	1.00	39.47
	ATOM	1049	CA	MET	A	437	17.257	17.087	5.975	1.00	38.20
	ATOM	1050	CB	MET	A	437	16.102	16.998	6.965	1.00	39.79
	ATOM	1051	C	MET	A	437	18.550	16.594	6.626	1.00	41.15
	ATOM	1052	O	MET	A	437	19.303	17.378	7.201	1.00	40.20
45	ATOM	1053	N	MET	A	438	18.804	15.285	6.538	1.00	39.65
	ATOM	1054	CA	MET	A	438	20.011	14.693	7.117	1.00	39.70
	ATOM	1055	CB	MET	A	438	19.787	13.221	7.463	1.00	39.90
	ATOM	1056	CG	MET	A	438	18.694	12.938	8.460	1.00	41.94
	ATOM	1057	SD	MET	A	438	18.747	11.188	8.880	1.00	43.12
50	ATOM	1058	CE	MET	A	438	20.374	11.064	9.619	1.00	43.73
	ATOM	1059	C	MET	A	438	21.176	14.756	6.142	1.00	38.03
	ATOM	1060	O	MET	A	438	22.321	14.503	6.522	1.00	38.39
	ATOM	1061	N	ASN	A	439	20.886	15.070	4.895	1.00	37.64
	ATOM	1062	CA	ASN	A	439	21.924	15.118	3.895	1.00	35.68
55	ATOM	1063	CB	ASN	A	439	23.019	16.125	4.243	1.00	40.98
	ATOM	1064	CG	ASN	A	439	23.933	16.407	3.090	1.00	45.09
	ATOM	1065	OD1	ASN	A	439	23.528	16.295	1.934	1.00	47.16
	ATOM	1066	ND2	ASN	A	439	25.197	16.733	3.372	1.00	46.87
	ATOM	1067	C	ASN	A	439	22.552	13.732	3.739	1.00	31.06
60	ATOM	1068	O	ASN	A	439	23.764	13.581	3.649	1.00	29.54
	ATOM	1069	N	LEU	A	440	21.692	12.698	3.704	1.00	31.47

5	ATOM	1070	CA	LEU	A	440	22.161	11.326	3.579	1.00	31.63
	ATOM	1071	CB	LEU	A	440	20.991	10.344	3.380	1.00	33.05
	ATOM	1072	CG	LEU	A	440	21.451	8.886	3.209	1.00	37.07
	ATOM	1073	CD1	LEU	A	440	21.957	8.353	4.546	1.00	36.18
	ATOM	1074	CD2	LEU	A	440	20.318	8.032	2.682	1.00	32.33
10	ATOM	1075	C	LEU	A	440	23.146	11.161	2.435	1.00	32.10
	ATOM	1076	O	LEU	A	440	22.925	11.671	1.333	1.00	32.76
	ATOM	1077	N	GLN	A	441	24.225	10.450	2.702	1.00	32.54
	ATOM	1078	CA	GLN	A	441	25.255	10.220	1.699	1.00	31.97
	ATOM	1079	CB	GLN	A	441	26.632	10.320	2.345	1.00	31.75
15	ATOM	1080	CG	GLN	A	441	26.896	11.669	2.979	1.00	35.56
	ATOM	1081	CD	GLN	A	441	27.040	12.748	1.939	1.00	34.97
	ATOM	1082	OE1	GLN	A	441	27.985	12.782	1.167	1.00	35.51
	ATOM	1083	NE2	GLN	A	441	26.053	13.659	1.899	1.00	35.41
	ATOM	1084	C	GLN	A	441	25.100	8.860	1.038	1.00	34.08
20	ATOM	1085	O	GLN	A	441	24.540	7.931	1.625	1.00	30.73
	ATOM	1086	N	GLY	A	442	25.608	8.752	-0.187	1.00	32.78
	ATOM	1087	CA	GLY	A	442	25.528	7.503	-0.921	1.00	32.91
	ATOM	1088	C	GLY	A	442	26.181	6.350	-0.184	1.00	31.87
	ATOM	1089	O	GLY	A	442	25.642	5.245	-0.154	1.00	33.18
25	ATOM	1090	N	GLU	A	443	27.340	6.603	0.416	1.00	30.60
	ATOM	1091	CA	GLU	A	443	28.057	5.567	1.150	1.00	30.85
	ATOM	1092	CB	GLU	A	443	29.376	6.111	1.704	1.00	32.74
	ATOM	1093	CG	GLU	A	443	30.425	6.378	0.646	1.00	36.30
	ATOM	1094	CD	GLU	A	443	30.310	7.770	0.066	1.00	40.92
30	ATOM	1095	OE1	GLU	A	443	29.677	8.630	0.716	1.00	42.27
	ATOM	1096	OE2	GLU	A	443	30.853	8.003	-1.038	1.00	46.82
	ATOM	1097	C	GLU	A	443	27.206	5.048	2.299	1.00	30.43
	ATOM	1098	O	GLU	A	443	27.211	3.854	2.595	1.00	28.11
	ATOM	1099	N	GLU	A	444	26.482	5.955	2.948	1.00	30.26
35	ATOM	1100	CA	GLU	A	444	25.619	5.589	4.067	1.00	28.18
	ATOM	1101	CB	GLU	A	444	25.147	6.843	4.797	1.00	26.32
	ATOM	1102	CG	GLU	A	444	26.250	7.633	5.463	1.00	29.27
	ATOM	1103	CD	GLU	A	444	25.748	8.944	6.023	1.00	29.62
	ATOM	1104	OE1	GLU	A	444	25.006	9.652	5.304	1.00	32.00
40	ATOM	1105	OE2	GLU	A	444	26.088	9.268	7.182	1.00	29.02
	ATOM	1106	C	GLU	A	444	24.403	4.813	3.572	1.00	26.93
	ATOM	1107	O	GLU	A	444	23.970	3.841	4.191	1.00	24.78
	ATOM	1108	N	PHE	A	445	23.861	5.256	2.443	1.00	27.79
	ATOM	1109	CA	PHE	A	445	22.688	4.633	1.853	1.00	24.50
45	ATOM	1110	CB	PHE	A	445	22.254	5.416	0.610	1.00	25.40
	ATOM	1111	CG	PHE	A	445	21.372	4.634	-0.316	1.00	23.74
	ATOM	1112	CD1	PHE	A	445	20.034	4.419	-0.004	1.00	23.00
	ATOM	1113	CD2	PHE	A	445	21.885	4.094	-1.489	1.00	22.37
	ATOM	1114	CE1	PHE	A	445	19.215	3.670	-0.855	1.00	22.57
50	ATOM	1115	CE2	PHE	A	445	21.079	3.349	-2.342	1.00	21.69
	ATOM	1116	CZ	PHE	A	445	19.741	3.138	-2.023	1.00	22.25
	ATOM	1117	C	PHE	A	445	22.913	3.169	1.489	1.00	22.81
	ATOM	1118	O	PHE	A	445	22.083	2.316	1.796	1.00	22.92
	ATOM	1119	N	VAL	A	446	24.019	2.868	0.822	1.00	22.46
55	ATOM	1120	CA	VAL	A	446	24.278	1.481	0.447	1.00	22.26
	ATOM	1121	CB	VAL	A	446	25.522	1.360	-0.465	1.00	22.87
	ATOM	1122	CG1	VAL	A	446	25.251	2.046	-1.799	1.00	22.57
	ATOM	1123	CG2	VAL	A	446	26.735	1.968	0.217	1.00	22.38
	ATOM	1124	C	VAL	A	446	24.467	0.614	1.694	1.00	23.68
60	ATOM	1125	O	VAL	A	446	24.177	-0.586	1.680	1.00	22.91
	ATOM	1126	N	CYS	A	447	24.962	1.223	2.770	1.00	22.02

5	ATOM	1127	CA	CYS	A	447	25.155	0.503	4.025	1.00	24.17
	ATOM	1128	CB	CYS	A	447	25.953	1.359	5.011	1.00	23.95
	ATOM	1129	SG	CYS	A	447	27.738	1.324	4.731	1.00	28.57
	ATOM	1130	C	CYS	A	447	23.781	0.178	4.618	1.00	21.14
	ATOM	1131	O	CYS	A	447	23.512	-0.960	5.002	1.00	19.37
10	ATOM	1132	N	LEU	A	448	22.915	1.186	4.680	1.00	19.28
	ATOM	1133	CA	LEU	A	448	21.568	1.002	5.219	1.00	21.31
	ATOM	1134	CB	LEU	A	448	20.803	2.324	5.207	1.00	21.90
	ATOM	1135	CG	LEU	A	448	21.142	3.337	6.303	1.00	26.61
	ATOM	1136	CD1	LEU	A	448	20.328	4.594	6.072	1.00	27.74
15	ATOM	1137	CD2	LEU	A	448	20.827	2.760	7.672	1.00	24.03
	ATOM	1138	C	LEU	A	448	20.766	-0.038	4.442	1.00	21.72
	ATOM	1139	O	LEU	A	448	20.006	-0.803	5.030	1.00	20.87
	ATOM	1140	N	LYS	A	449	20.929	-0.055	3.119	1.00	21.42
	ATOM	1141	CA	LYS	A	449	20.205	-0.997	2.269	1.00	20.98
20	ATOM	1142	CB	LYS	A	449	20.440	-0.659	0.788	1.00	21.55
	ATOM	1143	CG	LYS	A	449	19.438	-1.297	-0.173	1.00	24.82
	ATOM	1144	CD	LYS	A	449	19.456	-0.613	-1.542	1.00	23.33
	ATOM	1145	CE	LYS	A	449	20.816	-0.754	-2.229	1.00	23.58
	ATOM	1146	NZ	LYS	A	449	20.741	-0.482	-3.698	1.00	28.77
25	ATOM	1147	C	LYS	A	449	20.629	-2.436	2.548	1.00	20.33
	ATOM	1148	O	LYS	A	449	19.800	-3.345	2.552	1.00	20.57
	ATOM	1149	N	SER	A	450	21.924	-2.637	2.777	1.00	19.25
	ATOM	1150	CA	SER	A	450	22.451	-3.965	3.074	1.00	21.84
	ATOM	1151	CB	SER	A	450	23.982	-3.953	3.041	1.00	20.59
30	ATOM	1152	OG	SER	A	450	24.460	-3.975	1.702	1.00	29.78
	ATOM	1153	C	SER	A	450	21.975	-4.408	4.454	1.00	21.58
	ATOM	1154	O	SER	A	450	21.728	-5.590	4.682	1.00	20.06
	ATOM	1155	N	ILE	A	451	21.853	-3.449	5.369	1.00	22.20
	ATOM	1156	CA	ILE	A	451	21.385	-3.741	6.726	1.00	22.82
35	ATOM	1157	CB	ILE	A	451	21.452	-2.476	7.616	1.00	19.62
	ATOM	1158	CG2	ILE	A	451	20.593	-2.658	8.886	1.00	21.11
	ATOM	1159	CG1	ILE	A	451	22.909	-2.210	7.999	1.00	22.20
	ATOM	1160	CD1	ILE	A	451	23.115	-0.960	8.850	1.00	24.48
	ATOM	1161	C	ILE	A	451	19.952	-4.250	6.662	1.00	21.82
40	ATOM	1162	O	ILE	A	451	19.575	-5.184	7.369	1.00	21.72
	ATOM	1163	N	ILE	A	452	19.152	-3.642	5.795	1.00	20.18
	ATOM	1164	CA	ILE	A	452	17.763	-4.058	5.649	1.00	18.13
	ATOM	1165	CB	ILE	A	452	17.024	-3.145	4.627	1.00	19.72
	ATOM	1166	CG2	ILE	A	452	15.720	-3.792	4.169	1.00	18.99
45	ATOM	1167	CG1	ILE	A	452	16.725	-1.788	5.282	1.00	18.33
	ATOM	1168	CD1	ILE	A	452	16.284	-0.707	4.306	1.00	23.25
	ATOM	1169	C	ILE	A	452	17.725	-5.517	5.191	1.00	19.50
	ATOM	1170	O	ILE	A	452	16.980	-6.340	5.737	1.00	17.60
	ATOM	1171	N	LEU	A	453	18.555	-5.844	4.209	1.00	19.23
50	ATOM	1172	CA	LEU	A	453	18.589	-7.205	3.679	1.00	21.60
	ATOM	1173	CB	LEU	A	453	19.624	-7.316	2.554	1.00	21.50
	ATOM	1174	CG	LEU	A	453	19.835	-8.729	1.989	1.00	25.06
	ATOM	1175	CD1	LEU	A	453	18.550	-9.250	1.364	1.00	25.27
	ATOM	1176	CD2	LEU	A	453	20.948	-8.694	0.953	1.00	24.73
55	ATOM	1177	C	LEU	A	453	18.906	-8.245	4.746	1.00	19.41
	ATOM	1178	O	LEU	A	453	18.198	-9.241	4.891	1.00	20.75
	ATOM	1179	N	LEU	A	454	19.966	-7.997	5.499	1.00	21.35
	ATOM	1180	CA	LEU	A	454	20.410	-8.925	6.530	1.00	23.67
	ATOM	1181	CB	LEU	A	454	21.870	-8.625	6.878	1.00	20.69
60	ATOM	1182	CG	LEU	A	454	22.816	-8.584	5.673	1.00	24.92
	ATOM	1183	CD1	LEU	A	454	24.222	-8.268	6.132	1.00	24.27

							22.785	-9.913	4.952	1.00	22.84
5	ATOM	1184	CD2	LEU	A	454	19.572	-8.945	7.807	1.00	26.06
	ATOM	1185	C	LEU	A	454	19.413	-9.997	8.438	1.00	27.44
	ATOM	1186	O	LEU	A	454	19.011	-7.795	8.167	1.00	25.01
	ATOM	1187	N	ASN	A	455	18.240	-7.681	9.400	1.00	26.10
	ATOM	1188	CA	ASN	A	455	18.439	-6.295	10.002	1.00	22.67
10	ATOM	1189	CB	ASN	A	455	17.627	-6.109	11.264	1.00	26.67
	ATOM	1190	CG	ASN	A	455	17.899	-6.751	12.270	1.00	25.16
	ATOM	1191	OD1	ASN	A	455	16.615	-5.246	11.212	1.00	20.73
	ATOM	1192	ND2	ASN	A	455	16.739	-7.957	9.418	1.00	25.78
	ATOM	1193	C	ASN	A	455	16.230	-8.516	10.380	1.00	29.22
15	ATOM	1194	O	ASN	A	455	16.027	-7.549	8.381	1.00	28.51
	ATOM	1195	N	SER	A	456	14.578	-7.704	8.371	1.00	32.52
	ATOM	1196	CA	SER	A	456	14.019	-7.213	7.033	1.00	35.98
	ATOM	1197	CB	SER	A	456	14.266	-5.818	6.897	1.00	30.88
	ATOM	1198	OG	SER	A	456	14.033	-9.086	8.711	1.00	33.00
20	ATOM	1199	C	SER	A	456	13.112	-9.202	9.523	1.00	33.07
	ATOM	1200	O	SER	A	456	14.597	-10.130	8.117	1.00	28.40
	ATOM	1201	N	GLY	A	457	14.115	-11.464	8.413	1.00	36.28
	ATOM	1202	CA	GLY	A	457	15.055	-12.289	9.277	1.00	40.41
	ATOM	1203	C	GLY	A	457	14.831	-13.486	9.456	1.00	38.20
25	ATOM	1204	O	GLY	A	457	16.095	-11.657	9.820	1.00	44.13
	ATOM	1205	N	VAL	A	458	17.079	-12.356	10.647	1.00	51.09
	ATOM	1206	CA	VAL	A	458	18.214	-11.399	11.095	1.00	51.06
	ATOM	1207	CB	VAL	A	458	17.688	-10.390	12.104	1.00	51.75
	ATOM	1208	CG1	VAL	A	458	19.365	-12.199	11.692	1.00	50.65
30	ATOM	1209	CG2	VAL	A	458	16.513	-13.060	11.885	1.00	57.26
	ATOM	1210	C	VAL	A	458	17.085	-14.045	12.356	1.00	58.77
	ATOM	1211	O	VAL	A	458	15.401	-12.560	12.416	1.00	62.31
	ATOM	1212	N	TYR	A	459	14.793	-13.177	13.592	1.00	68.49
	ATOM	1213	CA	TYR	A	459	14.293	-12.100	14.560	1.00	70.46
35	ATOM	1214	CB	TYR	A	459	15.396	-11.196	15.069	1.00	71.73
	ATOM	1215	CG	TYR	A	459	15.127	-9.888	15.462	1.00	71.93
	ATOM	1216	CD1	TYR	A	459	16.147	-9.045	15.898	1.00	72.60
	ATOM	1217	CE1	TYR	A	459	16.716	-11.644	15.128	1.00	72.77
	ATOM	1218	CD2	TYR	A	459	17.741	-10.812	15.560	1.00	73.55
40	ATOM	1219	CE2	TYR	A	459	17.450	-9.514	15.941	1.00	72.93
	ATOM	1220	CZ	TYR	A	459	18.467	-8.687	16.351	1.00	74.56
	ATOM	1221	OH	TYR	A	459	13.649	-14.097	13.187	1.00	71.86
	ATOM	1222	C	TYR	A	459	13.380	-15.099	13.852	1.00	73.11
	ATOM	1223	O	TYR	A	459	12.981	-13.756	12.090	1.00	74.84
45	ATOM	1224	N	THR	A	460	11.881	-14.567	11.589	1.00	77.66
	ATOM	1225	CA	THR	A	460	11.246	-13.900	10.373	1.00	76.69
	ATOM	1226	CB	THR	A	460	12.436	-15.938	11.212	1.00	80.26
	ATOM	1227	C	THR	A	460	11.684	-16.866	10.912	1.00	80.82
	ATOM	1228	O	THR	A	460	13.762	-16.051	11.231	1.00	82.69
50	ATOM	1229	N	PHE	A	461	14.440	-17.299	10.905	1.00	85.63
	ATOM	1230	CA	PHE	A	461	15.920	-17.034	10.630	1.00	85.47
	ATOM	1231	CB	PHE	A	461	14.284	-18.288	12.059	1.00	87.52
	ATOM	1232	C	PHE	A	461	14.493	-17.940	13.224	1.00	86.53
	ATOM	1233	O	PHE	A	461	13.914	-19.520	11.724	1.00	89.49
55	ATOM	1234	N	LEU	A	462	13.711	-20.568	12.718	1.00	91.34
	ATOM	1235	CA	LEU	A	462	12.961	-21.741	12.087	1.00	91.23
	ATOM	1236	CB	LEU	A	462	15.016	-21.060	13.340	1.00	92.05
	ATOM	1237	C	LEU	A	462	16.042	-21.165	12.664	1.00	91.91
	ATOM	1238	O	LEU	A	462	14.966	-21.357	14.635	1.00	92.53
60	ATOM	1239	N	SER	A	463	16.131	-21.855	15.358	1.00	92.96
	ATOM	1240	CA	SER	A	463					



5	ATOM	1241	CB	SER	A	463	16.033	-21.483	16.833	1.00	91.67
	ATOM	1242	C	SER	A	463	16.189	-23.371	15.200	1.00	93.39
	ATOM	1243	O	SER	A	463	15.156	-24.034	15.102	1.00	93.44
	ATOM	1244	N	SER	A	464	17.399	-23.917	15.167	1.00	93.82
	ATOM	1245	CA	SER	A	464	17.577	-25.355	15.015	1.00	93.85
10	ATOM	1246	CB	SER	A	464	17.284	-25.769	13.577	1.00	93.74
	ATOM	1247	C	SER	A	464	18.997	-25.743	15.396	1.00	93.96
	ATOM	1248	O	SER	A	464	19.815	-26.074	14.535	1.00	93.65
	ATOM	1249	N	THR	A	465	19.279	-25.699	16.694	1.00	93.91
	ATOM	1250	CA	THR	A	465	20.600	-26.036	17.212	1.00	93.79
15	ATOM	1251	CB	THR	A	465	20.952	-27.483	16.863	1.00	93.38
	ATOM	1252	C	THR	A	465	21.640	-25.085	16.634	1.00	93.27
	ATOM	1253	O	THR	A	465	21.302	-24.017	16.121	1.00	93.03
	ATOM	1254	N	LEU	A	466	22.907	-25.479	16.723	1.00	93.26
	ATOM	1255	CA	LEU	A	466	23.999	-24.665	16.207	1.00	92.34
20	ATOM	1256	CB	LEU	A	466	25.335	-25.338	16.498	1.00	91.59
	ATOM	1257	C	LEU	A	466	23.829	-24.461	14.706	1.00	92.18
	ATOM	1258	O	LEU	A	466	24.411	-23.545	14.125	1.00	92.67
	ATOM	1259	N	LYS	A	467	23.028	-25.323	14.086	1.00	91.28
	ATOM	1260	CA	LYS	A	467	22.772	-25.238	12.653	1.00	90.02
25	ATOM	1261	CB	LYS	A	467	21.740	-26.287	12.240	1.00	89.93
	ATOM	1262	C	LYS	A	467	22.269	-23.841	12.308	1.00	88.35
	ATOM	1263	O	LYS	A	467	23.032	-22.990	11.849	1.00	88.50
	ATOM	1264	N	SER	A	468	20.981	-23.610	12.536	1.00	86.02
	ATOM	1265	CA	SER	A	468	20.384	-22.315	12.252	1.00	84.10
30	ATOM	1266	CB	SER	A	468	18.901	-22.333	12.620	1.00	84.08
	ATOM	1267	OG	SER	A	468	18.229	-23.378	11.937	1.00	83.03
	ATOM	1268	C	SER	A	468	21.109	-21.230	13.040	1.00	83.39
	ATOM	1269	O	SER	A	468	21.264	-20.105	12.565	1.00	83.48
	ATOM	1270	N	LEU	A	469	21.558	-21.579	14.242	1.00	82.04
35	ATOM	1271	CA	LEU	A	469	22.276	-20.640	15.098	1.00	80.28
	ATOM	1272	CB	LEU	A	469	22.595	-21.294	16.436	1.00	79.81
	ATOM	1273	C	LEU	A	469	23.564	-20.174	14.419	1.00	79.18
	ATOM	1274	O	LEU	A	469	24.111	-19.122	14.756	1.00	78.61
	ATOM	1275	N	GLU	A	470	24.044	-20.969	13.466	1.00	76.69
40	ATOM	1276	CA	GLU	A	470	25.256	-20.638	12.726	1.00	74.84
	ATOM	1277	CB	GLU	A	470	25.803	-21.880	12.032	1.00	74.12
	ATOM	1278	C	GLU	A	470	24.920	-19.565	11.697	1.00	73.77
	ATOM	1279	O	GLU	A	470	25.617	-18.556	11.581	1.00	72.94
	ATOM	1280	N	GLU	A	471	23.842	-19.792	10.953	1.00	72.08
45	ATOM	1281	CA	GLU	A	471	23.396	-18.842	9.945	1.00	70.05
	ATOM	1282	CB	GLU	A	471	22.461	-19.526	8.944	1.00	71.52
	ATOM	1283	CG	GLU	A	471	23.150	-19.976	7.668	1.00	72.90
	ATOM	1284	CD	GLU	A	471	24.512	-20.586	7.932	1.00	74.01
	ATOM	1285	OE1	GLU	A	471	25.469	-20.258	7.198	1.00	74.22
50	ATOM	1286	OE2	GLU	A	471	24.626	-21.395	8.878	1.00	75.18
	ATOM	1287	C	GLU	A	471	22.667	-17.692	10.630	1.00	67.33
	ATOM	1288	O	GLU	A	471	21.685	-17.165	10.107	1.00	67.77
	ATOM	1289	N	LYS	A	472	23.152	-17.319	11.811	1.00	62.63
	ATOM	1290	CA	LYS	A	472	22.564	-16.229	12.578	1.00	57.41
55	ATOM	1291	CB	LYS	A	472	21.697	-16.777	13.713	1.00	58.74
	ATOM	1292	CG	LYS	A	472	20.683	-15.776	14.243	1.00	60.32
	ATOM	1293	CD	LYS	A	472	19.271	-16.342	14.219	1.00	60.73
	ATOM	1294	CE	LYS	A	472	18.485	-15.909	15.449	1.00	61.78
	ATOM	1295	NZ	LYS	A	472	19.352	-15.788	16.658	1.00	60.09
60	ATOM	1296	C	LYS	A	472	23.662	-15.339	13.150	1.00	53.42
	ATOM	1297	O	LYS	A	472	23.631	-14.120	12.978	1.00	50.87

5	ATOM	1298	N	ASP	A	473	24.628	-15.949	13.830	1.00	47.52
	ATOM	1299	CA	ASP	A	473	25.732	-15.194	14.405	1.00	45.55
	ATOM	1300	CB	ASP	A	473	26.613	-16.094	15.269	1.00	50.48
	ATOM	1301	CG	ASP	A	473	26.380	-15.885	16.749	1.00	55.50
	ATOM	1302	OD1	ASP	A	473	25.272	-15.436	17.118	1.00	58.06
10	ATOM	1303	OD2	ASP	A	473	27.304	-16.170	17.541	1.00	59.81
	ATOM	1304	C	ASP	A	473	26.557	-14.611	13.269	1.00	42.62
	ATOM	1305	O	ASP	A	473	27.087	-13.506	13.373	1.00	42.10
	ATOM	1306	N	HIS	A	474	26.663	-15.364	12.180	1.00	38.05
	ATOM	1307	CA	HIS	A	474	27.416	-14.904	11.026	1.00	37.25
15	ATOM	1308	CB	HIS	A	474	27.429	-15.978	9.941	1.00	35.07
	ATOM	1309	CG	HIS	A	474	28.036	-15.523	8.653	1.00	37.36
	ATOM	1310	CD2	HIS	A	474	29.292	-15.113	8.355	1.00	38.86
	ATOM	1311	ND1	HIS	A	474	27.322	-15.452	7.476	1.00	41.31
	ATOM	1312	CE1	HIS	A	474	28.110	-15.020	6.509	1.00	40.86
20	ATOM	1313	NE2	HIS	A	474	29.311	-14.807	7.016	1.00	44.49
	ATOM	1314	C	HIS	A	474	26.749	-13.640	10.493	1.00	36.68
	ATOM	1315	O	HIS	A	474	27.417	-12.676	10.132	1.00	36.48
	ATOM	1316	N	ILE	A	475	25.422	-13.652	10.447	1.00	35.93
	ATOM	1317	CA	ILE	A	475	24.683	-12.499	9.963	1.00	36.21
25	ATOM	1318	CB	ILE	A	475	23.174	-12.797	9.868	1.00	36.31
	ATOM	1319	CG2	ILE	A	475	22.411	-11.527	9.513	1.00	38.19
	ATOM	1320	CG1	ILE	A	475	22.922	-13.874	8.813	1.00	36.97
	ATOM	1321	CD1	ILE	A	475	21.528	-14.454	8.869	1.00	35.59
	ATOM	1322	C	ILE	A	475	24.893	-11.322	10.907	1.00	35.34
30	ATOM	1323	O	ILE	A	475	25.092	-10.189	10.471	1.00	33.20
	ATOM	1324	N	HIS	A	476	24.857	-11.596	12.206	1.00	35.95
	ATOM	1325	CA	HIS	A	476	25.031	-10.540	13.193	1.00	35.06
	ATOM	1326	CB	HIS	A	476	24.681	-11.062	14.585	1.00	37.30
	ATOM	1327	CG	HIS	A	476	23.210	-11.068	14.860	1.00	43.06
35	ATOM	1328	CD2	HIS	A	476	22.329	-10.051	15.017	1.00	43.93
	ATOM	1329	ND1	HIS	A	476	22.476	-12.230	14.968	1.00	45.60
	ATOM	1330	CE1	HIS	A	476	21.207	-11.928	15.177	1.00	47.56
	ATOM	1331	NE2	HIS	A	476	21.091	-10.613	15.211	1.00	46.21
	ATOM	1332	C	HIS	A	476	26.438	-9.966	13.170	1.00	35.40
40	ATOM	1333	O	HIS	A	476	26.634	-8.774	13.415	1.00	35.45
	ATOM	1334	N	ARG	A	477	27.420	-10.805	12.862	1.00	34.07
	ATOM	1335	CA	ARG	A	477	28.796	-10.331	12.795	1.00	34.18
	ATOM	1336	CB	ARG	A	477	29.757	-11.506	12.605	1.00	41.04
	ATOM	1337	CG	ARG	A	477	29.800	-12.459	13.788	1.00	47.61
45	ATOM	1338	CD	ARG	A	477	30.782	-13.599	13.557	1.00	55.67
	ATOM	1339	NE	ARG	A	477	31.780	-13.675	14.622	1.00	60.17
	ATOM	1340	CZ	ARG	A	477	32.780	-12.811	14.770	1.00	61.98
	ATOM	1341	NH1	ARG	A	477	32.918	-11.803	13.918	1.00	64.29
	ATOM	1342	NH2	ARG	A	477	33.643	-12.955	15.766	1.00	62.79
50	ATOM	1343	C	ARG	A	477	28.906	-9.361	11.621	1.00	30.77
	ATOM	1344	O	ARG	A	477	29.462	-8.268	11.753	1.00	33.59
	ATOM	1345	N	VAL	A	478	28.369	-9.766	10.475	1.00	27.65
	ATOM	1346	CA	VAL	A	478	28.389	-8.930	9.280	1.00	27.07
	ATOM	1347	CB	VAL	A	478	27.658	-9.605	8.100	1.00	28.00
55	ATOM	1348	CG1	VAL	A	478	27.672	-8.678	6.890	1.00	25.83
	ATOM	1349	CG2	VAL	A	478	28.319	-10.933	7.761	1.00	31.66
	ATOM	1350	C	VAL	A	478	27.689	-7.610	9.584	1.00	26.92
	ATOM	1351	O	VAL	A	478	28.216	-6.536	9.294	1.00	26.97
	ATOM	1352	N	LEU	A	479	26.499	-7.702	10.171	1.00	25.74
60	ATOM	1353	CA	LEU	A	479	25.727	-6.516	10.530	1.00	27.97
	ATOM	1354	CB	LEU	A	479	24.474	-6.912	11.324	1.00	25.55

5	ATOM	1355	CG	LEU	A	479	23.211	-7.229	10.517	1.00	29.01
	ATOM	1356	CD1	LEU	A	479	22.056	-7.503	11.481	1.00	27.05
	ATOM	1357	CD2	LEU	A	479	22.864	-6.063	9.584	1.00	24.92
	ATOM	1358	C	LEU	A	479	26.592	-5.582	11.369	1.00	25.39
	ATOM	1359	O	LEU	A	479	26.595	-4.370	11.158	1.00	27.39
10	ATOM	1360	N	ASP	A	480	27.324	-6.158	12.320	1.00	26.04
	ATOM	1361	CA	ASP	A	480	28.206	-5.388	13.193	1.00	27.32
	ATOM	1362	CB	ASP	A	480	28.878	-6.305	14.222	1.00	26.67
	ATOM	1363	CG	ASP	A	480	27.990	-6.602	15.417	1.00	31.02
	ATOM	1364	OD1	ASP	A	480	28.355	-7.505	16.198	1.00	31.50
15	ATOM	1365	OD2	ASP	A	480	26.935	-5.944	15.580	1.00	32.21
	ATOM	1366	C	ASP	A	480	29.283	-4.699	12.361	1.00	25.59
	ATOM	1367	O	ASP	A	480	29.672	-3.562	12.636	1.00	27.15
	ATOM	1368	N	LYS	A	481	29.767	-5.394	11.340	1.00	25.17
	ATOM	1369	CA	LYS	A	481	30.794	-4.830	10.477	1.00	24.93
20	ATOM	1370	CB	LYS	A	481	31.306	-5.890	9.512	1.00	28.42
	ATOM	1371	CG	LYS	A	481	32.158	-6.953	10.188	1.00	35.59
	ATOM	1372	CD	LYS	A	481	32.894	-7.799	9.157	1.00	41.21
	ATOM	1373	CE	LYS	A	481	33.883	-6.963	8.350	1.00	41.48
	ATOM	1374	NZ	LYS	A	481	34.954	-6.388	9.215	1.00	43.22
25	ATOM	1375	C	LYS	A	481	30.260	-3.635	9.696	1.00	26.12
	ATOM	1376	O	LYS	A	481	30.979	-2.657	9.463	1.00	23.73
	ATOM	1377	N	ILE	A	482	28.996	-3.705	9.291	1.00	25.44
	ATOM	1378	CA	ILE	A	482	28.421	-2.598	8.545	1.00	27.69
	ATOM	1379	CB	ILE	A	482	27.066	-2.983	7.915	1.00	27.59
30	ATOM	1380	CG2	ILE	A	482	26.470	-1.788	7.183	1.00	25.97
	ATOM	1381	CG1	ILE	A	482	27.274	-4.131	6.922	1.00	23.80
	ATOM	1382	CD1	ILE	A	482	26.000	-4.838	6.533	1.00	21.30
	ATOM	1383	C	ILE	A	482	28.253	-1.408	9.481	1.00	27.33
	ATOM	1384	O	ILE	A	482	28.312	-0.256	9.045	1.00	28.55
35	ATOM	1385	N	THR	A	483	28.046	-1.690	10.768	1.00	25.03
	ATOM	1386	CA	THR	A	483	27.905	-0.632	11.760	1.00	23.62
	ATOM	1387	CB	THR	A	483	27.535	-1.192	13.154	1.00	22.18
	ATOM	1388	OG1	THR	A	483	26.181	-1.658	13.133	1.00	25.39
	ATOM	1389	CG2	THR	A	483	27.673	-0.111	14.226	1.00	25.84
40	ATOM	1390	C	THR	A	483	29.257	0.074	11.858	1.00	23.04
	ATOM	1391	O	THR	A	483	29.331	1.306	11.846	1.00	23.55
	ATOM	1392	N	ASP	A	484	30.324	-0.714	11.960	1.00	22.24
	ATOM	1393	CA	ASP	A	484	31.674	-0.152	12.039	1.00	25.48
	ATOM	1394	CB	ASP	A	484	32.718	-1.273	12.107	1.00	26.88
45	ATOM	1395	CG	ASP	A	484	32.629	-2.083	13.394	1.00	32.52
	ATOM	1396	OD1	ASP	A	484	32.002	-1.608	14.366	1.00	33.68
	ATOM	1397	OD2	ASP	A	484	33.185	-3.198	13.434	1.00	34.63
	ATOM	1398	C	ASP	A	484	31.930	0.715	10.807	1.00	25.16
	ATOM	1399	O	ASP	A	484	32.481	1.812	10.905	1.00	26.05
50	ATOM	1400	N	THR	A	485	31.505	0.226	9.645	1.00	28.96
	ATOM	1401	CA	THR	A	485	31.689	0.960	8.394	1.00	26.63
	ATOM	1402	CB	THR	A	485	31.124	0.166	7.197	1.00	26.12
	ATOM	1403	OG1	THR	A	485	31.753	-1.123	7.132	1.00	24.30
	ATOM	1404	CG2	THR	A	485	31.381	0.907	5.898	1.00	23.31
55	ATOM	1405	C	THR	A	485	30.994	2.318	8.468	1.00	28.90
	ATOM	1406	O	THR	A	485	31.583	3.354	8.137	1.00	27.26
	ATOM	1407	N	LEU	A	486	29.743	2.310	8.915	1.00	24.76
	ATOM	1408	CA	LEU	A	486	28.973	3.537	9.027	1.00	26.19
	ATOM	1409	CB	LEU	A	486	27.567	3.233	9.547	1.00	27.27
60	ATOM	1410	CG	LEU	A	486	26.508	2.921	8.486	1.00	23.50
	ATOM	1411	CD1	LEU	A	486	25.210	2.550	9.183	1.00	22.03

							26.309	4.128	7.577	1.00	21.35
5	ATOM	1412	CD2	LEU	A	486	29.662	4.519	9.960	1.00	27.36
	ATOM	1413	C	LEU	A	486	29.745	5.710	9.669	1.00	25.87
	ATOM	1414	O	LEU	A	486	30.151	4.015	11.088	1.00	27.88
	ATOM	1415	N	ILE	A	487	30.843	4.857	12.055	1.00	28.40
	ATOM	1416	CA	ILE	A	487	31.203	4.054	13.332	1.00	26.74
10	ATOM	1417	CB	ILE	A	487	32.255	4.803	14.154	1.00	27.54
	ATOM	1418	CG2	ILE	A	487	29.937	3.813	14.163	1.00	25.93
	ATOM	1419	CG1	ILE	A	487	29.237	5.088	14.624	1.00	23.42
	ATOM	1420	CD1	ILE	A	487	32.125	5.393	11.412	1.00	28.89
	ATOM	1421	C	ILE	A	487	32.497	6.554	11.602	1.00	29.85
15	ATOM	1422	O	ILE	A	487	32.791	4.533	10.649	1.00	29.71
	ATOM	1423	N	HIS	A	488	34.031	4.898	9.967	1.00	34.12
	ATOM	1424	CA	HIS	A	488	34.585	3.691	9.207	1.00	36.61
	ATOM	1425	CB	HIS	A	488	35.799	3.997	8.385	1.00	42.74
	ATOM	1426	CG	HIS	A	488	35.970	4.089	7.045	1.00	43.12
20	ATOM	1427	CD2	HIS	A	488	37.034	4.239	8.946	1.00	43.13
	ATOM	1428	ND1	HIS	A	488	37.913	4.466	7.987	1.00	43.40
	ATOM	1429	CE1	HIS	A	488	37.293	4.381	6.825	1.00	45.63
	ATOM	1430	NE2	HIS	A	488	33.799	6.051	8.998	1.00	32.74
	ATOM	1431	C	HIS	A	488	34.577	7.004	8.955	1.00	31.06
25	ATOM	1432	O	HIS	A	488	32.721	5.958	8.223	1.00	33.56
	ATOM	1433	N	LEU	A	489	32.384	6.992	7.258	1.00	30.78
	ATOM	1434	CA	LEU	A	489	31.145	6.587	6.464	1.00	34.67
	ATOM	1435	CB	LEU	A	489	31.310	5.353	5.574	1.00	34.73
	ATOM	1436	CG	LEU	A	489	29.945	4.856	5.125	1.00	33.21
30	ATOM	1437	CD1	LEU	A	489	32.183	5.701	4.378	1.00	35.92
	ATOM	1438	CD2	LEU	A	489	32.124	8.320	7.954	1.00	33.97
	ATOM	1439	C	LEU	A	489	32.587	9.365	7.507	1.00	33.22
	ATOM	1440	O	LEU	A	489	31.387	8.274	9.058	1.00	31.33
	ATOM	1441	N	MET	A	490	31.056	9.482	9.801	1.00	30.61
35	ATOM	1442	CA	MET	A	490	30.000	9.161	10.862	1.00	32.34
	ATOM	1443	CB	MET	A	490	28.607	8.940	10.289	1.00	30.71
	ATOM	1444	CG	MET	A	490	27.457	8.247	11.496	1.00	31.14
	ATOM	1445	SD	MET	A	490	26.321	7.408	10.418	1.00	30.36
	ATOM	1446	CE	MET	A	490	32.287	10.108	10.455	1.00	32.22
40	ATOM	1447	C	MET	A	490	32.412	11.330	10.517	1.00	28.25
	ATOM	1448	O	MET	A	490	33.184	9.262	10.949	1.00	33.81
	ATOM	1449	N	ALA	A	491	34.407	9.730	11.585	1.00	39.92
	ATOM	1450	CA	ALA	A	491	35.168	8.554	12.185	1.00	37.22
	ATOM	1451	CB	ALA	A	491	35.275	10.445	10.550	1.00	42.68
45	ATOM	1452	C	ALA	A	491	35.865	11.487	10.838	1.00	45.32
	ATOM	1453	O	ALA	A	491	35.339	9.876	9.347	1.00	44.39
	ATOM	1454	N	LYS	A	492	36.122	10.440	8.248	1.00	44.80
	ATOM	1455	CA	LYS	A	492	36.136	9.477	7.052	1.00	46.96
	ATOM	1456	CB	LYS	A	492	37.490	8.840	6.744	1.00	47.20
50	ATOM	1457	CG	LYS	A	492	37.390	7.830	5.595	1.00	45.71
	ATOM	1458	CD	LYS	A	492	38.631	6.937	5.518	1.00	45.55
	ATOM	1459	CE	LYS	A	492	38.357	5.577	4.948	1.00	36.28
	ATOM	1460	NZ	LYS	A	492	35.534	11.780	7.809	1.00	45.61
	ATOM	1461	C	LYS	A	492	36.227	12.604	7.215	1.00	46.18
55	ATOM	1462	O	LYS	A	492	34.254	11.992	8.100	1.00	43.75
	ATOM	1463	N	ALA	A	493	33.590	13.238	7.728	1.00	42.42
	ATOM	1464	CA	ALA	A	493	32.097	13.001	7.528	1.00	40.92
	ATOM	1465	CB	ALA	A	493	33.816	14.305	8.796	1.00	41.78
	ATOM	1466	C	ALA	A	493	33.277	15.410	8.707	1.00	40.76
60	ATOM	1467	O	ALA	A	493	34.604	13.960	9.811	1.00	41.01
	ATOM	1468	N	GLY	A	494					

5	ATOM	1469	CA	GLY	A	494	34.903	14.904	10.873	1.00	41.63
	ATOM	1470	C	GLY	A	494	33.857	15.060	11.965	1.00	41.18
	ATOM	1471	O	GLY	A	494	33.916	16.011	12.747	1.00	38.22
	ATOM	1472	N	LEU	A	495	32.905	14.138	12.043	1.00	39.53
	ATOM	1473	CA	LEU	A	495	31.876	14.248	13.068	1.00	38.91
10	ATOM	1474	CB	LEU	A	495	30.713	13.304	12.769	1.00	39.20
	ATOM	1475	CG	LEU	A	495	29.540	13.901	11.988	1.00	40.73
	ATOM	1476	CD1	LEU	A	495	29.976	14.170	10.553	1.00	37.80
	ATOM	1477	CD2	LEU	A	495	28.349	12.943	12.026	1.00	40.94
	ATOM	1478	C	LEU	A	495	32.461	13.923	14.431	1.00	36.01
15	ATOM	1479	O	LEU	A	495	33.347	13.074	14.544	1.00	34.85
	ATOM	1480	N	THR	A	496	31.979	14.604	15.459	1.00	37.52
	ATOM	1481	CA	THR	A	496	32.462	14.350	16.812	1.00	35.45
	ATOM	1482	CB	THR	A	496	31.925	15.375	17.829	1.00	37.55
	ATOM	1483	OG1	THR	A	496	30.498	15.263	17.908	1.00	32.93
20	ATOM	1484	CG2	THR	A	496	32.315	16.797	17.434	1.00	36.16
	ATOM	1485	C	THR	A	496	31.933	12.987	17.210	1.00	35.67
	ATOM	1486	O	THR	A	496	31.081	12.427	16.521	1.00	34.34
	ATOM	1487	N	LEU	A	497	32.429	12.452	18.319	1.00	34.88
	ATOM	1488	CA	LEU	A	497	31.965	11.151	18.786	1.00	35.67
25	ATOM	1489	CB	LEU	A	497	32.689	10.760	20.074	1.00	41.10
	ATOM	1490	CG	LEU	A	497	33.714	9.640	19.896	1.00	45.27
	ATOM	1491	CD1	LEU	A	497	34.755	9.692	21.008	1.00	45.09
	ATOM	1492	CD2	LEU	A	497	32.988	8.305	19.884	1.00	47.77
	ATOM	1493	C	LEU	A	497	30.455	11.198	19.026	1.00	33.72
30	ATOM	1494	O	LEU	A	497	29.712	10.350	18.534	1.00	33.20
	ATOM	1495	N	GLN	A	498	30.006	12.202	19.773	1.00	30.82
	ATOM	1496	CA	GLN	A	498	28.586	12.348	20.062	1.00	31.47
	ATOM	1497	CB	GLN	A	498	28.344	13.566	20.951	1.00	30.51
	ATOM	1498	CG	GLN	A	498	26.894	13.796	21.341	1.00	34.38
35	ATOM	1499	CD	GLN	A	498	26.712	15.130	22.015	1.00	38.60
	ATOM	1500	OE1	GLN	A	498	27.363	16.112	21.686	1.00	42.92
	ATOM	1501	NE2	GLN	A	498	25.809	15.176	23.008	1.00	40.02
	ATOM	1502	C	GLN	A	498	27.776	12.476	18.773	1.00	30.47
	ATOM	1503	O	GLN	A	498	26.682	11.927	18.665	1.00	30.85
40	ATOM	1504	N	GLN	A	499	28.311	13.196	17.793	1.00	29.52
	ATOM	1505	CA	GLN	A	499	27.603	13.362	16.524	1.00	30.24
	ATOM	1506	CB	GLN	A	499	28.292	14.420	15.661	1.00	30.20
	ATOM	1507	CG	GLN	A	499	28.135	15.840	16.191	1.00	31.60
	ATOM	1508	CD	GLN	A	499	28.930	16.849	15.389	1.00	31.61
45	ATOM	1509	OE1	GLN	A	499	29.956	16.518	14.795	1.00	30.66
	ATOM	1510	NE2	GLN	A	499	28.457	18.089	15.364	1.00	34.17
	ATOM	1511	C	GLN	A	499	27.529	12.047	15.753	1.00	29.40
	ATOM	1512	O	GLN	A	499	26.567	11.793	15.032	1.00	30.04
	ATOM	1513	N	GLN	A	500	28.550	11.214	15.903	1.00	25.67
50	ATOM	1514	CA	GLN	A	500	28.577	9.937	15.216	1.00	29.30
	ATOM	1515	CB	GLN	A	500	29.933	9.276	15.406	1.00	31.52
	ATOM	1516	CG	GLN	A	500	31.012	9.839	14.508	1.00	33.05
	ATOM	1517	CD	GLN	A	500	32.371	9.370	14.930	1.00	34.84
	ATOM	1518	OE1	GLN	A	500	32.612	8.194	15.141	1.00	36.47
55	ATOM	1519	NE2	GLN	A	500	33.301	10.324	15.082	1.00	38.25
	ATOM	1520	C	GLN	A	500	27.459	9.017	15.711	1.00	27.98
	ATOM	1521	O	GLN	A	500	26.700	8.469	14.908	1.00	24.84
	ATOM	1522	N	HIS	A	501	27.357	8.864	17.029	1.00	26.20
	ATOM	1523	CA	HIS	A	501	26.327	8.021	17.631	1.00	27.63
60	ATOM	1524	CB	HIS	A	501	26.535	7.919	19.145	1.00	27.97
	ATOM	1525	CG	HIS	A	501	27.892	7.420	19.535	1.00	34.27

5	ATOM	1526	CD2	HIS	A	501	28.726	6.540	18.931	1.00	36.10
	ATOM	1527	ND1	HIS	A	501	28.541	7.844	20.676	1.00	31.81
	ATOM	1528	CE1	HIS	A	501	29.716	7.244	20.758	1.00	34.89
	ATOM	1529	NE2	HIS	A	501	29.854	6.448	19.712	1.00	37.46
	ATOM	1530	C	HIS	A	501	24.935	8.572	17.348	1.00	24.93
10	ATOM	1531	O	HIS	A	501	23.998	7.815	17.107	1.00	26.73
	ATOM	1532	N	GLN	A	502	24.796	9.892	17.379	1.00	22.79
	ATOM	1533	CA	GLN	A	502	23.504	10.498	17.119	1.00	26.14
	ATOM	1534	CB	GLN	A	502	23.554	12.006	17.371	1.00	22.36
	ATOM	1535	CG	GLN	A	502	23.460	12.378	18.848	1.00	26.19
15	ATOM	1536	CD	GLN	A	502	23.589	13.875	19.089	1.00	28.67
	ATOM	1537	OE1	GLN	A	502	23.632	14.663	18.149	1.00	28.40
	ATOM	1538	NE2	GLN	A	502	23.651	14.268	20.355	1.00	24.72
	ATOM	1539	C	GLN	A	502	23.056	10.221	15.685	1.00	26.19
	ATOM	1540	O	GLN	A	502	21.913	9.822	15.453	1.00	24.09
20	ATOM	1541	N	ARG	A	503	23.955	10.429	14.727	1.00	24.88
	ATOM	1542	CA	ARG	A	503	23.630	10.196	13.326	1.00	25.25
	ATOM	1543	CB	ARG	A	503	24.772	10.668	12.418	1.00	27.63
	ATOM	1544	CG	ARG	A	503	24.432	10.563	10.932	1.00	28.75
	ATOM	1545	CD	ARG	A	503	25.479	11.222	10.056	1.00	27.72
25	ATOM	1546	NE	ARG	A	503	25.072	11.214	8.654	1.00	29.35
	ATOM	1547	CZ	ARG	A	503	24.279	12.126	8.105	1.00	25.84
	ATOM	1548	NH1	ARG	A	503	23.804	13.120	8.840	1.00	27.35
	ATOM	1549	NH2	ARG	A	503	23.962	12.044	6.820	1.00	30.63
	ATOM	1550	C	ARG	A	503	23.347	8.716	13.065	1.00	24.53
30	ATOM	1551	O	ARG	A	503	22.425	8.375	12.321	1.00	25.90
	ATOM	1552	N	LEU	A	504	24.143	7.841	13.672	1.00	23.00
	ATOM	1553	CA	LEU	A	504	23.953	6.406	13.496	1.00	22.60
	ATOM	1554	CB	LEU	A	504	24.971	5.621	14.323	1.00	25.43
	ATOM	1555	CG	LEU	A	504	24.781	4.100	14.344	1.00	25.23
35	ATOM	1556	CD1	LEU	A	504	25.166	3.505	12.991	1.00	28.52
	ATOM	1557	CD2	LEU	A	504	25.627	3.495	15.444	1.00	22.14
	ATOM	1558	C	LEU	A	504	22.541	6.030	13.934	1.00	22.84
	ATOM	1559	O	LEU	A	504	21.846	5.288	13.245	1.00	21.51
	ATOM	1560	N	ALA	A	505	22.120	6.547	15.083	1.00	20.16
40	ATOM	1561	CA	ALA	A	505	20.784	6.262	15.585	1.00	21.08
	ATOM	1562	CB	ALA	A	505	20.605	6.868	16.980	1.00	23.57
	ATOM	1563	C	ALA	A	505	19.738	6.832	14.628	1.00	20.20
	ATOM	1564	O	ALA	A	505	18.754	6.164	14.293	1.00	17.31
	ATOM	1565	N	GLN	A	506	19.954	8.066	14.184	1.00	22.11
45	ATOM	1566	CA	GLN	A	506	19.013	8.711	13.277	1.00	21.70
	ATOM	1567	CB	GLN	A	506	19.502	10.111	12.903	1.00	22.26
	ATOM	1568	CG	GLN	A	506	19.240	11.158	13.975	1.00	25.84
	ATOM	1569	CD	GLN	A	506	20.187	12.333	13.857	1.00	32.88
	ATOM	1570	OE1	GLN	A	506	20.704	12.614	12.777	1.00	31.23
50	ATOM	1571	NE2	GLN	A	506	20.423	13.025	14.968	1.00	32.97
	ATOM	1572	C	GLN	A	506	18.813	7.881	12.016	1.00	23.57
	ATOM	1573	O	GLN	A	506	17.684	7.715	11.550	1.00	21.83
	ATOM	1574	N	LEU	A	507	19.905	7.354	11.474	1.00	19.98
	ATOM	1575	CA	LEU	A	507	19.827	6.537	10.263	1.00	22.03
55	ATOM	1576	CB	LEU	A	507	21.231	6.244	9.725	1.00	23.02
	ATOM	1577	CG	LEU	A	507	22.026	7.457	9.225	1.00	25.80
	ATOM	1578	CD1	LEU	A	507	23.371	6.994	8.713	1.00	27.67
	ATOM	1579	CD2	LEU	A	507	21.264	8.176	8.130	1.00	25.62
	ATOM	1580	C	LEU	A	507	19.090	5.219	10.496	1.00	22.35
60	ATOM	1581	O	LEU	A	507	18.242	4.825	9.695	1.00	19.33
	ATOM	1582	N	LEU	A	508	19.402	4.539	11.592	1.00	21.29

5	ATOM	1583	CA	LEU	A	508	18.755	3.260	11.881	1.00	20.72
	ATOM	1584	CB	LEU	A	508	19.501	2.535	13.001	1.00	22.29
	ATOM	1585	CG	LEU	A	508	20.977	2.311	12.678	1.00	24.70
	ATOM	1586	CD1	LEU	A	508	21.642	1.551	13.814	1.00	21.37
	ATOM	1587	CD2	LEU	A	508	21.095	1.542	11.367	1.00	27.88
10	ATOM	1588	C	LEU	A	508	17.279	3.396	12.239	1.00	19.14
	ATOM	1589	O	LEU	A	508	16.498	2.478	12.003	1.00	17.80
	ATOM	1590	N	LEU	A	509	16.895	4.530	12.815	1.00	19.23
	ATOM	1591	CA	LEU	A	509	15.495	4.747	13.173	1.00	20.14
	ATOM	1592	CB	LEU	A	509	15.347	6.030	13.999	1.00	20.28
15	ATOM	1593	CG	LEU	A	509	15.710	5.858	15.479	1.00	21.35
	ATOM	1594	CD1	LEU	A	509	15.354	7.106	16.263	1.00	19.29
	ATOM	1595	CD2	LEU	A	509	14.989	4.656	16.038	1.00	20.84
	ATOM	1596	C	LEU	A	509	14.681	4.841	11.885	1.00	21.69
	ATOM	1597	O	LEU	A	509	13.493	4.514	11.854	1.00	22.40
20	ATOM	1598	N	ILE	A	510	15.343	5.270	10.815	1.00	20.22
	ATOM	1599	CA	ILE	A	510	14.710	5.397	9.508	1.00	20.40
	ATOM	1600	CB	ILE	A	510	15.720	5.946	8.464	1.00	28.34
	ATOM	1601	CG2	ILE	A	510	15.208	5.710	7.056	1.00	32.54
	ATOM	1602	CG1	ILE	A	510	15.965	7.438	8.696	1.00	28.23
25	ATOM	1603	CD1	ILE	A	510	14.789	8.189	9.288	1.00	33.16
	ATOM	1604	C	ILE	A	510	14.210	4.025	9.049	1.00	23.21
	ATOM	1605	O	ILE	A	510	13.120	3.906	8.474	1.00	21.16
	ATOM	1606	N	LEU	A	511	14.998	2.989	9.323	1.00	18.38
	ATOM	1607	CA	LEU	A	511	14.633	1.634	8.917	1.00	20.10
30	ATOM	1608	CB	LEU	A	511	15.754	0.656	9.267	1.00	21.69
	ATOM	1609	CG	LEU	A	511	17.128	1.022	8.692	1.00	26.03
	ATOM	1610	CD1	LEU	A	511	18.024	-0.206	8.724	1.00	22.68
	ATOM	1611	CD2	LEU	A	511	16.996	1.544	7.267	1.00	26.00
	ATOM	1612	C	LEU	A	511	13.326	1.181	9.543	1.00	18.51
35	ATOM	1613	O	LEU	A	511	12.663	0.283	9.025	1.00	17.40
	ATOM	1614	N	SER	A	512	12.963	1.799	10.664	1.00	18.68
	ATOM	1615	CA	SER	A	512	11.718	1.471	11.331	1.00	18.67
	ATOM	1616	CB	SER	A	512	11.661	2.117	12.720	1.00	18.58
	ATOM	1617	OG	SER	A	512	10.315	2.229	13.165	1.00	27.92
40	ATOM	1618	C	SER	A	512	10.572	1.994	10.464	1.00	18.43
	ATOM	1619	O	SER	A	512	9.584	1.296	10.236	1.00	13.91
	ATOM	1620	N	HIS	A	513	10.713	3.228	9.982	1.00	18.95
	ATOM	1621	CA	HIS	A	513	9.698	3.831	9.124	1.00	20.82
	ATOM	1622	CB	HIS	A	513	10.013	5.315	8.894	1.00	24.36
45	ATOM	1623	CG	HIS	A	513	9.923	6.146	10.136	1.00	32.13
	ATOM	1624	CD2	HIS	A	513	8.863	6.744	10.734	1.00	35.29
	ATOM	1625	ND1	HIS	A	513	11.010	6.391	10.949	1.00	35.00
	ATOM	1626	CE1	HIS	A	513	10.624	7.101	11.995	1.00	34.67
	ATOM	1627	NE2	HIS	A	513	9.326	7.328	11.889	1.00	35.82
50	ATOM	1628	C	HIS	A	513	9.650	3.079	7.790	1.00	19.08
	ATOM	1629	O	HIS	A	513	8.575	2.863	7.220	1.00	21.20
	ATOM	1630	N	ILE	A	514	10.809	2.662	7.297	1.00	15.58
	ATOM	1631	CA	ILE	A	514	10.849	1.921	6.038	1.00	16.48
	ATOM	1632	CB	ILE	A	514	12.312	1.678	5.576	1.00	20.09
55	ATOM	1633	CG2	ILE	A	514	12.349	0.602	4.499	1.00	19.55
	ATOM	1634	CG1	ILE	A	514	12.891	2.986	5.019	1.00	22.62
	ATOM	1635	CD1	ILE	A	514	14.393	2.992	4.874	1.00	27.34
	ATOM	1636	C	ILE	A	514	10.112	0.590	6.210	1.00	16.40
	ATOM	1637	O	ILE	A	514	9.364	0.164	5.328	1.00	17.91
60	ATOM	1638	N	ARG	A	515	10.301	-0.071	7.347	1.00	18.20
	ATOM	1639	CA	ARG	A	515	9.585	-1.327	7.564	1.00	18.05

5	ATOM	1640	CB	ARG	A	515	9.984	-1.980	8.889	1.00	18.36
	ATOM	1641	CG	ARG	A	515	9.173	-3.237	9.213	1.00	17.84
	ATOM	1642	CD	ARG	A	515	9.823	-4.470	8.606	1.00	17.94
	ATOM	1643	NE	ARG	A	515	11.038	-4.813	9.334	1.00	26.96
	ATOM	1644	CZ	ARG	A	515	11.406	-6.051	9.641	1.00	25.13
10	ATOM	1645	NH1	ARG	A	515	10.654	-7.080	9.281	1.00	23.49
	ATOM	1646	NH2	ARG	A	515	12.511	-6.254	10.340	1.00	32.16
	ATOM	1647	C	ARG	A	515	8.089	-1.020	7.594	1.00	18.29
	ATOM	1648	O	ARG	A	515	7.275	-1.759	7.038	1.00	16.22
	ATOM	1649	N	HIS	A	516	7.726	0.085	8.237	1.00	19.33
15	ATOM	1650	CA	HIS	A	516	6.317	0.441	8.330	1.00	17.78
	ATOM	1651	CB	HIS	A	516	6.126	1.702	9.166	1.00	16.84
	ATOM	1652	CG	HIS	A	516	4.692	2.101	9.312	1.00	18.16
	ATOM	1653	CD2	HIS	A	516	3.967	3.061	8.691	1.00	21.17
	ATOM	1654	ND1	HIS	A	516	3.830	1.469	10.180	1.00	20.70
20	ATOM	1655	CE1	HIS	A	516	2.633	2.022	10.089	1.00	21.52
	ATOM	1656	NE2	HIS	A	516	2.689	2.992	9.191	1.00	20.16
	ATOM	1657	C	HIS	A	516	5.708	0.659	6.954	1.00	16.63
	ATOM	1658	O	HIS	A	516	4.598	0.216	6.689	1.00	18.58
	ATOM	1659	N	MET	A	517	6.438	1.334	6.073	1.00	15.29
25	ATOM	1660	CA	MET	A	517	5.925	1.589	4.730	1.00	16.58
	ATOM	1661	CB	MET	A	517	6.837	2.576	4.002	1.00	18.66
	ATOM	1662	CG	MET	A	517	6.805	3.978	4.631	1.00	16.88
	ATOM	1663	SD	MET	A	517	7.670	5.243	3.701	1.00	24.08
	ATOM	1664	CE	MET	A	517	9.390	4.777	3.962	1.00	14.30
30	ATOM	1665	C	MET	A	517	5.773	0.289	3.940	1.00	17.86
	ATOM	1666	O	MET	A	517	4.791	0.101	3.224	1.00	18.25
	ATOM	1667	N	SER	A	518	6.741	-0.610	4.086	1.00	17.43
	ATOM	1668	CA	SER	A	518	6.697	-1.896	3.403	1.00	18.40
	ATOM	1669	CB	SER	A	518	7.974	-2.695	3.680	1.00	16.77
35	ATOM	1670	OG	SER	A	518	7.834	-4.030	3.227	1.00	24.23
	ATOM	1671	C	SER	A	518	5.476	-2.695	3.854	1.00	17.91
	ATOM	1672	O	SER	A	518	4.788	-3.295	3.030	1.00	18.97
	ATOM	1673	N	ASN	A	519	5.204	-2.697	5.159	1.00	21.82
	ATOM	1674	CA	ASN	A	519	4.047	-3.418	5.696	1.00	21.99
40	ATOM	1675	CB	ASN	A	519	3.957	-3.257	7.216	1.00	23.24
	ATOM	1676	CG	ASN	A	519	5.046	-4.011	7.957	1.00	31.14
	ATOM	1677	OD1	ASN	A	519	5.585	-4.999	7.461	1.00	32.50
	ATOM	1678	ND2	ASN	A	519	5.368	-3.545	9.163	1.00	29.10
	ATOM	1679	C	ASN	A	519	2.761	-2.871	5.079	1.00	23.76
45	ATOM	1680	O	ASN	A	519	1.902	-3.632	4.631	1.00	24.48
	ATOM	1681	N	LYS	A	520	2.627	-1.548	5.078	1.00	20.58
	ATOM	1682	CA	LYS	A	520	1.449	-0.900	4.512	1.00	25.49
	ATOM	1683	CB	LYS	A	520	1.484	0.607	4.786	1.00	24.73
	ATOM	1684	CG	LYS	A	520	1.512	0.996	6.264	1.00	32.31
50	ATOM	1685	CD	LYS	A	520	0.656	0.080	7.133	1.00	37.11
	ATOM	1686	CE	LYS	A	520	-0.787	0.547	7.181	1.00	41.56
	ATOM	1687	NZ	LYS	A	520	-1.560	-0.134	8.261	1.00	42.66
	ATOM	1688	C	LYS	A	520	1.380	-1.144	3.005	1.00	25.40
	ATOM	1689	O	LYS	A	520	0.316	-1.436	2.467	1.00	26.44
55	ATOM	1690	N	GLY	A	521	2.520	-1.021	2.332	1.00	22.88
	ATOM	1691	CA	GLY	A	521	2.561	-1.236	0.897	1.00	21.53
	ATOM	1692	C	GLY	A	521	2.177	-2.655	0.536	1.00	24.79
	ATOM	1693	O	GLY	A	521	1.426	-2.878	-0.413	1.00	25.71
	ATOM	1694	N	MET	A	522	2.696	-3.619	1.290	1.00	22.75
60	ATOM	1695	CA	MET	A	522	2.393	-5.027	1.058	1.00	23.40
	ATOM	1696	CB	MET	A	522	3.170	-5.898	2.042	1.00	25.74



5	ATOM	1697	CG	MET	A	522	3.396	-7.308	1.559	1.00	31.06
	ATOM	1698	SD	MET	A	522	4.572	-7.352	0.202	1.00	34.06
	ATOM	1699	CE	MET	A	522	6.125	-7.229	1.113	1.00	29.28
	ATOM	1700	C	MET	A	522	0.893	-5.281	1.218	1.00	26.49
	ATOM	1701	O	MET	A	522	0.268	-5.920	0.361	1.00	25.47
10	ATOM	1702	N	GLU	A	523	0.321	-4.790	2.318	1.00	24.95
	ATOM	1703	CA	GLU	A	523	-1.110	-4.954	2.566	1.00	27.15
	ATOM	1704	CB	GLU	A	523	-1.555	-4.206	3.835	1.00	31.08
	ATOM	1705	CG	GLU	A	523	-0.830	-4.564	5.124	1.00	38.93
	ATOM	1706	CD	GLU	A	523	-1.153	-3.585	6.258	1.00	46.90
15	ATOM	1707	OE1	GLU	A	523	-2.225	-2.938	6.200	1.00	47.40
	ATOM	1708	OE2	GLU	A	523	-0.337	-3.460	7.202	1.00	47.39
	ATOM	1709	C	GLU	A	523	-1.872	-4.368	1.381	1.00	26.10
	ATOM	1710	O	GLU	A	523	-2.817	-4.964	0.882	1.00	24.25
	ATOM	1711	N	HIS	A	524	-1.449	-3.182	0.940	1.00	24.74
20	ATOM	1712	CA	HIS	A	524	-2.093	-2.505	-0.173	1.00	26.17
	ATOM	1713	CB	HIS	A	524	-1.481	-1.125	-0.379	1.00	24.64
	ATOM	1714	CG	HIS	A	524	-2.233	-0.278	-1.355	1.00	30.59
	ATOM	1715	CD2	HIS	A	524	-3.227	0.624	-1.172	1.00	32.15
	ATOM	1716	ND1	HIS	A	524	-2.008	-0.332	-2.713	1.00	27.46
25	ATOM	1717	CE1	HIS	A	524	-2.829	0.502	-3.326	1.00	34.58
	ATOM	1718	NE2	HIS	A	524	-3.580	1.094	-2.413	1.00	30.50
	ATOM	1719	C	HIS	A	524	-1.996	-3.294	-1.474	1.00	28.06
	ATOM	1720	O	HIS	A	524	-2.976	-3.419	-2.217	1.00	29.81
	ATOM	1721	N	LEU	A	525	-0.811	-3.824	-1.746	1.00	27.07
30	ATOM	1722	CA	LEU	A	525	-0.594	-4.601	-2.955	1.00	29.30
	ATOM	1723	CB	LEU	A	525	0.865	-5.039	-3.051	1.00	26.39
	ATOM	1724	CG	LEU	A	525	1.307	-5.765	-4.321	1.00	29.34
	ATOM	1725	CD1	LEU	A	525	0.734	-5.076	-5.562	1.00	29.61
	ATOM	1726	CD2	LEU	A	525	2.829	-5.769	-4.370	1.00	29.22
35	ATOM	1727	C	LEU	A	525	-1.497	-5.822	-2.950	1.00	31.67
	ATOM	1728	O	LEU	A	525	-2.128	-6.133	-3.957	1.00	32.45
	ATOM	1729	N	TYR	A	526	-1.559	-6.512	-1.814	1.00	36.14
	ATOM	1730	CA	TYR	A	526	-2.397	-7.698	-1.696	1.00	40.36
	ATOM	1731	CB	TYR	A	526	-2.221	-8.350	-0.324	1.00	45.27
40	ATOM	1732	CG	TYR	A	526	-2.849	-9.722	-0.229	1.00	50.62
	ATOM	1733	CD1	TYR	A	526	-2.114	-10.867	-0.537	1.00	54.55
	ATOM	1734	CE1	TYR	A	526	-2.698	-12.136	-0.482	1.00	57.27
	ATOM	1735	CD2	TYR	A	526	-4.188	-9.876	0.142	1.00	53.48
	ATOM	1736	CE2	TYR	A	526	-4.781	-11.141	0.201	1.00	55.93
45	ATOM	1737	CZ	TYR	A	526	-4.029	-12.264	-0.113	1.00	56.60
	ATOM	1738	OH	TYR	A	526	-4.603	-13.515	-0.063	1.00	60.70
	ATOM	1739	C	TYR	A	526	-3.852	-7.298	-1.893	1.00	42.83
	ATOM	1740	O	TYR	A	526	-4.673	-8.094	-2.349	1.00	43.49
	ATOM	1741	N	SER	A	527	-4.158	-6.055	-1.543	1.00	41.55
50	ATOM	1742	CA	SER	A	527	-5.503	-5.523	-1.686	1.00	44.04
	ATOM	1743	CB	SER	A	527	-5.606	-4.169	-0.979	1.00	43.47
	ATOM	1744	OG	SER	A	527	-6.954	-3.789	-0.786	1.00	47.51
	ATOM	1745	C	SER	A	527	-5.817	-5.356	-3.172	1.00	44.18
	ATOM	1746	O	SER	A	527	-6.883	-5.757	-3.642	1.00	44.88
55	ATOM	1747	N	MET	A	528	-4.883	-4.755	-3.901	1.00	41.79
	ATOM	1748	CA	MET	A	528	-5.047	-4.536	-5.331	1.00	44.04
	ATOM	1749	CB	MET	A	528	-3.898	-3.679	-5.870	1.00	44.78
	ATOM	1750	CG	MET	A	528	-3.965	-2.206	-5.468	1.00	45.37
	ATOM	1751	SD	MET	A	528	-5.652	-1.598	-5.273	1.00	51.83
60	ATOM	1752	CE	MET	A	528	-5.553	-0.004	-6.044	1.00	46.61
	ATOM	1753	C	MET	A	528	-5.087	-5.871	-6.071	1.00	44.29

							-5.689	-5.979	-7.137	1.00	44.02
5	ATOM	1754	O	MET	A	528	-4.443	-6.883	-5.499	1.00	46.78
	ATOM	1755	N	LYS	A	529	-4.413	-8.213	-6.099	1.00	51.28
	ATOM	1756	CA	LYS	A	529	-3.550	-9.158	-5.261	1.00	50.87
	ATOM	1757	CB	LYS	A	529	-2.798	-10.204	-6.071	1.00	50.55
	ATOM	1758	CG	LYS	A	529	-3.548	-11.520	-6.104	1.00	51.25
10	ATOM	1759	CD	LYS	A	529	-2.616	-12.694	-5.856	1.00	53.22
	ATOM	1760	CE	LYS	A	529	-2.420	-12.954	-4.402	1.00	53.22
	ATOM	1761	NZ	LYS	A	529	-5.829	-8.768	-6.182	1.00	54.27
	ATOM	1762	C	LYS	A	529	-6.325	-9.069	-7.266	1.00	55.50
	ATOM	1763	O	LYS	A	529	-6.472	-8.901	-5.027	1.00	56.71
15	ATOM	1764	N	CYS	A	530	-7.833	-9.416	-4.961	1.00	58.35
	ATOM	1765	CA	CYS	A	530	-8.333	-9.380	-3.517	1.00	59.78
	ATOM	1766	CB	CYS	A	530	-7.289	-10.304	-2.358	1.00	63.19
	ATOM	1767	SG	CYS	A	530	-8.766	-8.609	-5.858	1.00	59.36
	ATOM	1768	C	CYS	A	530	-9.644	-9.169	-6.514	1.00	59.52
20	ATOM	1769	O	CYS	A	530	-8.569	-7.293	-5.888	1.00	59.24
	ATOM	1770	N	LYS	A	531	-9.390	-6.411	-6.713	1.00	60.14
	ATOM	1771	CA	LYS	A	531	-9.158	-4.952	-6.317	1.00	58.92
	ATOM	1772	CB	LYS	A	531	-9.073	-6.615	-8.195	1.00	61.48
	ATOM	1773	C	LYS	A	531	-9.618	-5.928	-9.061	1.00	61.74
25	ATOM	1774	O	LYS	A	531	-8.179	-7.561	-8.474	1.00	61.65
	ATOM	1775	N	ASN	A	532	-7.783	-7.890	-9.840	1.00	61.60
	ATOM	1776	CA	ASN	A	532	-8.966	-8.518	-10.581	1.00	62.28
	ATOM	1777	CB	ASN	A	532	-8.750	-9.985	-10.878	1.00	64.66
	ATOM	1778	CG	ASN	A	532	-8.344	-10.352	-11.983	1.00	67.08
30	ATOM	1779	OD1	ASN	A	532	-9.016	-10.836	-9.891	1.00	62.68
	ATOM	1780	ND2	ASN	A	532	-7.247	-6.710	-10.648	1.00	59.75
	ATOM	1781	C	ASN	A	532	-7.487	-6.615	-11.850	1.00	57.50
	ATOM	1782	O	ASN	A	532	-6.507	-5.822	-9.992	1.00	59.39
	ATOM	1783	N	VAL	A	533	-5.954	-4.656	-10.669	1.00	58.22
35	ATOM	1784	CA	VAL	A	533	-6.223	-3.371	-9.865	1.00	59.20
	ATOM	1785	CB	VAL	A	533	-6.181	-2.163	-10.785	1.00	59.21
	ATOM	1786	CG1	VAL	A	533	-7.574	-3.467	-9.172	1.00	59.57
	ATOM	1787	CG2	VAL	A	533	-4.452	-4.767	-10.907	1.00	57.86
	ATOM	1788	C	VAL	A	533	-3.846	-3.874	-11.499	1.00	60.56
40	ATOM	1789	O	VAL	A	533	-3.852	-5.863	-10.451	1.00	56.03
	ATOM	1790	N	VAL	A	534	-2.417	-6.063	-10.621	1.00	54.11
	ATOM	1791	CA	VAL	A	534	-1.767	-6.632	-9.341	1.00	54.02
	ATOM	1792	CB	VAL	A	534	-0.300	-6.950	-9.601	1.00	52.37
	ATOM	1793	CG1	VAL	A	534	-1.900	-5.635	-8.200	1.00	55.70
45	ATOM	1794	CG2	VAL	A	534	-2.089	-7.008	-11.770	1.00	54.31
	ATOM	1795	C	VAL	A	534	-2.519	-8.164	-11.780	1.00	51.66
	ATOM	1796	O	VAL	A	534	-1.315	-6.527	-12.755	1.00	53.54
	ATOM	1797	N	PRO	A	535	-0.749	-5.172	-12.874	1.00	54.28
	ATOM	1798	CD	PRO	A	535	-0.949	-7.373	-13.893	1.00	53.24
50	ATOM	1799	CA	PRO	A	535	0.011	-6.500	-14.697	1.00	52.71
	ATOM	1800	CB	PRO	A	535	-0.353	-5.102	-14.319	1.00	53.19
	ATOM	1801	CG	PRO	A	535	-0.296	-8.664	-13.411	1.00	54.25
	ATOM	1802	C	PRO	A	535	0.121	-8.768	-12.254	1.00	54.56
	ATOM	1803	O	PRO	A	535	-0.203	-9.645	-14.299	1.00	53.63
55	ATOM	1804	N	LEU	A	536	0.382	-10.926	-13.937	1.00	53.11
	ATOM	1805	CA	LEU	A	536	-0.250	-12.046	-14.763	1.00	51.88
	ATOM	1806	CB	LEU	A	536	-0.686	-13.256	-13.938	1.00	51.83
	ATOM	1807	CG	LEU	A	536	-1.953	-12.917	-13.173	1.00	49.51
	ATOM	1808	CD1	LEU	A	536	-0.905	-14.449	-14.854	1.00	53.43
60	ATOM	1809	CD2	LEU	A	536	1.895	-10.990	-14.081	1.00	52.58
	ATOM	1810	C	LEU	A	536					

5	ATOM	1811	O	LEU	A	536	2.414	-11.501-15.075	1.00	55.33
	ATOM	1812	N	TYR	A	537	2.601	-10.462-13.087	1.00	48.72
	ATOM	1813	CA	TYR	A	537	4.057	-10.501-13.093	1.00	44.22
	ATOM	1814	CB	TYR	A	537	4.627	-9.134-12.709	1.00	44.52
	ATOM	1815	CG	TYR	A	537	4.331	-8.053-13.731	1.00	45.18
10	ATOM	1816	CD1	TYR	A	537	3.623	-6.905-13.376	1.00	43.77
	ATOM	1817	CE1	TYR	A	537	3.334	-5.915-14.317	1.00	45.23
	ATOM	1818	CD2	TYR	A	537	4.747	-8.187-15.058	1.00	46.91
	ATOM	1819	CE2	TYR	A	537	4.462	-7.202-16.008	1.00	43.93
	ATOM	1820	CZ	TYR	A	537	3.757	-6.071-15.631	1.00	46.70
15	ATOM	1821	OH	TYR	A	537	3.472	-5.097-16.565	1.00	48.35
	ATOM	1822	C	TYR	A	537	4.401	-11.562-12.056	1.00	41.29
	ATOM	1823	O	TYR	A	537	4.330	-11.319-10.856	1.00	41.82
	ATOM	1824	N	ASP	A	538	4.748	-12.748-12.540	1.00	40.34
	ATOM	1825	CA	ASP	A	538	5.055	-13.896-11.691	1.00	38.84
20	ATOM	1826	CB	ASP	A	538	5.594	-15.037-12.554	1.00	43.47
	ATOM	1827	CG	ASP	A	538	4.571	-15.531-13.566	1.00	47.67
	ATOM	1828	OD1	ASP	A	538	4.931	-16.373-14.416	1.00	49.33
	ATOM	1829	OD2	ASP	A	538	3.405	-15.073-13.511	1.00	48.07
	ATOM	1830	C	ASP	A	538	5.991	-13.676-10.508	1.00	37.28
25	ATOM	1831	O	ASP	A	538	5.620	-13.964 -9.371	1.00	38.55
	ATOM	1832	N	LEU	A	539	7.196	-13.200-10.766	1.00	33.83
	ATOM	1833	CA	LEU	A	539	8.155	-12.959 -9.692	1.00	32.80
	ATOM	1834	CB	LEU	A	539	9.419	-12.323-10.263	1.00	32.78
	ATOM	1835	CG	LEU	A	539	10.561	-12.031 -9.292	1.00	30.93
30	ATOM	1836	CD1	LEU	A	539	10.913	-13.280 -8.492	1.00	33.81
	ATOM	1837	CD2	LEU	A	539	11.758	-11.538-10.077	1.00	25.92
	ATOM	1838	C	LEU	A	539	7.558	-12.050 -8.614	1.00	31.85
	ATOM	1839	O	LEU	A	539	7.590	-12.367 -7.423	1.00	25.63
	ATOM	1840	N	LEU	A	540	7.011	-10.917 -9.042	1.00	32.07
35	ATOM	1841	CA	LEU	A	540	6.411	-9.976 -8.111	1.00	31.03
	ATOM	1842	CB	LEU	A	540	5.792	-8.800 -8.861	1.00	30.56
	ATOM	1843	CG	LEU	A	540	5.124	-7.774 -7.945	1.00	31.12
	ATOM	1844	CD1	LEU	A	540	6.092	-7.357 -6.838	1.00	29.76
	ATOM	1845	CD2	LEU	A	540	4.693	-6.572 -8.762	1.00	30.85
40	ATOM	1846	C	LEU	A	540	5.337	-10.660 -7.282	1.00	34.55
	ATOM	1847	O	LEU	A	540	5.316	-10.522 -6.063	1.00	31.60
	ATOM	1848	N	LEU	A	541	4.446	-11.388 -7.941	1.00	35.64
	ATOM	1849	CA	LEU	A	541	3.378	-12.101 -7.245	1.00	37.84
	ATOM	1850	CB	LEU	A	541	2.452	-12.771 -8.255	1.00	38.49
45	ATOM	1851	CG	LEU	A	541	1.244	-11.932 -8.678	1.00	39.80
	ATOM	1852	CD1	LEU	A	541	0.476	-11.476 -7.448	1.00	40.02
	ATOM	1853	CD2	LEU	A	541	1.713	-10.733 -9.485	1.00	40.48
	ATOM	1854	C	LEU	A	541	3.937	-13.147 -6.275	1.00	40.10
	ATOM	1855	O	LEU	A	541	3.472	-13.254 -5.137	1.00	42.72
50	ATOM	1856	N	GLU	A	542	4.929	-13.915 -6.723	1.00	38.45
	ATOM	1857	CA	GLU	A	542	5.535	-14.932 -5.868	1.00	39.59
	ATOM	1858	CB	GLU	A	542	6.738	-15.566 -6.564	1.00	41.73
	ATOM	1859	CG	GLU	A	542	6.396	-16.327 -7.831	1.00	48.34
	ATOM	1860	CD	GLU	A	542	6.931	-17.747 -7.819	1.00	52.57
55	ATOM	1861	OE1	GLU	A	542	8.049	-17.961 -7.298	1.00	52.70
	ATOM	1862	OE2	GLU	A	542	6.230	-18.647 -8.331	1.00	53.69
	ATOM	1863	C	GLU	A	542	5.989	-14.299 -4.553	1.00	39.94
	ATOM	1864	O	GLU	A	542	5.567	-14.710 -3.472	1.00	40.99
	ATOM	1865	N	MET	A	543	6.844	-13.287 -4.663	1.00	38.29
60	ATOM	1866	CA	MET	A	543	7.380	-12.580 -3.503	1.00	38.11
	ATOM	1867	CB	MET	A	543	8.242	-11.408 -3.963	1.00	37.34

5	ATOM	1868	CG	MET	A	543	9.311	-11.797	-4.953	1.00	40.59
	ATOM	1869	SD	MET	A	543	10.829	-12.223	-4.114	1.00	45.64
	ATOM	1870	CE	MET	A	543	12.014	-11.399	-5.151	1.00	42.61
	ATOM	1871	C	MET	A	543	6.287	-12.064	-2.581	1.00	37.94
10	ATOM	1872	O	MET	A	543	6.413	-12.127	-1.358	1.00	39.20
	ATOM	1873	N	LEU	A	544	5.218	-11.544	-3.175	1.00	39.44
	ATOM	1874	CA	LEU	A	544	4.100	-11.013	-2.408	1.00	40.91
	ATOM	1875	CB	LEU	A	544	3.087	-10.344	-3.341	1.00	39.88
15	ATOM	1876	CG	LEU	A	544	1.775	-9.905	-2.688	1.00	42.70
	ATOM	1877	CD1	LEU	A	544	2.060	-8.886	-1.586	1.00	37.35
	ATOM	1878	CD2	LEU	A	544	0.854	-9.317	-3.741	1.00	38.47
	ATOM	1879	C	LEU	A	544	3.420	-12.120	-1.614	1.00	42.83
20	ATOM	1880	O	LEU	A	544	2.957	-11.899	-0.496	1.00	42.73
	ATOM	1881	N	ASP	A	545	3.367	-13.313	-2.197	1.00	46.32
	ATOM	1882	CA	ASP	A	545	2.746	-14.456	-1.539	1.00	50.65
	ATOM	1883	CB	ASP	A	545	2.606	-15.617	-2.524	1.00	53.67
25	ATOM	1884	CG	ASP	A	545	1.703	-15.278	-3.691	1.00	57.35
	ATOM	1885	OD1	ASP	A	545	0.697	-14.568	-3.475	1.00	59.99
	ATOM	1886	OD2	ASP	A	545	1.999	-15.718	-4.824	1.00	59.68
	ATOM	1887	C	ASP	A	545	3.559	-14.898	-0.327	1.00	50.74
30	ATOM	1888	O	ASP	A	545	3.004	-15.388	0.657	1.00	49.39
	ATOM	1889	N	ALA	A	546	4.874	-14.723	-0.401	1.00	51.82
	ATOM	1890	CA	ALA	A	546	5.750	-15.095	0.702	1.00	53.12
	ATOM	1891	CB	ALA	A	546	7.180	-14.678	0.395	1.00	53.19
35	ATOM	1892	C	ALA	A	546	5.269	-14.424	1.987	1.00	54.67
	ATOM	1893	O	ALA	A	546	5.476	-14.940	3.085	1.00	52.32
	ATOM	1894	N	HIS	A	547	4.622	-13.270	1.838	1.00	56.66
	ATOM	1895	CA	HIS	A	547	4.102	-12.520	2.978	1.00	59.19
40	ATOM	1896	CB	HIS	A	547	4.144	-11.017	2.684	1.00	56.70
	ATOM	1897	CG	HIS	A	547	5.489	-10.394	2.896	1.00	54.64
	ATOM	1898	CD2	HIS	A	547	6.644	-10.506	2.199	1.00	53.92
	ATOM	1899	ND1	HIS	A	547	5.748	-9.514	3.925	1.00	52.17
45	ATOM	1900	CE1	HIS	A	547	7.004	-9.111	3.853	1.00	52.16
	ATOM	1901	NE2	HIS	A	547	7.570	-9.698	2.814	1.00	51.90
	ATOM	1902	C	HIS	A	547	2.668	-12.940	3.306	1.00	62.77
	ATOM	1903	O	HIS	A	547	2.668	-12.940	3.306	1.00	62.77
50	ATOM	1904	N	ARG	A	548	1.842	-12.120	3.707	1.00	63.24
	ATOM	1905	CA	ARG	A	548	1.842	-12.120	3.707	1.00	63.24
	ATOM	1906	CB	ARG	A	548	2.381	-14.224	3.133	1.00	68.37
	ATOM	1907	CG	ARG	A	548	2.381	-14.224	3.133	1.00	68.37
55	ATOM	1908	CD	ARG	A	548	1.053	-14.758	3.411	1.00	72.75
	ATOM	1909	NE	ARG	A	548	0.243	-14.864	2.113	1.00	73.73
	ATOM	1910	CZ	ARG	A	548	-1.149	-14.243	2.186	1.00	74.04
	ATOM	1911	NH1	ARG	A	548	-1.081	-12.728	2.297	1.00	74.50
60	ATOM	1912	NH2	ARG	A	548	-2.305	-12.167	2.863	1.00	75.04
	ATOM	1913	C	ARG	A	548	-2.478	-10.880	3.149	1.00	75.59
	ATOM	1914	O	ARG	A	548	-1.506	-10.006	2.919	1.00	75.79
	ATOM	1915	N	LEU	A	549	-3.627	-10.464	3.662	1.00	76.00
60	ATOM	1916	CA	LEU	A	549	1.179	-16.133	4.061	1.00	74.94
	ATOM	1917	CB	LEU	A	549	0.197	-16.697	4.549	1.00	75.15
	ATOM	1918	C	LEU	A	549	2.398	-16.665	4.063	1.00	76.49
	ATOM	1919	O	LEU	A	549	2.669	-17.969	4.653	1.00	78.14
60	ATOM	1920	OXT	LEU	A	549	2.971	-18.986	3.557	1.00	77.55
	HETATM	1921	CP9	DES	A	600	3.846	-17.870	5.619	1.00	79.13
	HETATM	1922	CP8	DES	A	600	4.892	-17.317	5.215	1.00	80.40
	HETATM	1923	CP7	DES	A	600	3.708	-18.341	6.769	1.00	79.46
60	HETATM	1924	CP6	DES	A	600	5.390	-3.061	-6.139	1.00	21.38
	HETATM	1924	CP6	DES	A	600	5.834	-1.989	-5.134	1.00	22.41
60	HETATM	1924	CP6	DES	A	600	5.038	-0.714	-5.236	1.00	21.32
	HETATM	1924	CP6	DES	A	600	3.587	-0.864	-5.062	1.00	25.87

5	HETATM	1925	CP1	DES	A	600	2.987	-0.978	-3.784	1.00	23.92
	HETATM	1926	CP2	DES	A	600	1.597	-1.150	-3.684	1.00	29.77
	HETATM	1927	CP3	DES	A	600	0.842	-1.214	-4.871	1.00	31.40
	HETATM	1928	OP3	DES	A	600	-0.506	-1.419	-4.824	1.00	33.36
	HETATM	1929	CP4	DES	A	600	1.421	-1.099	-6.143	1.00	27.01
10	HETATM	1930	CP5	DES	A	600	2.793	-0.929	-6.230	1.00	27.40
	HETATM	1931	C7	DES	A	600	5.671	0.461	-5.482	1.00	22.39
	HETATM	1932	C6	DES	A	600	7.113	0.561	-5.809	1.00	21.75
	HETATM	1933	C5	DES	A	600	7.541	0.306	-7.131	1.00	19.97
	HETATM	1934	C4	DES	A	600	8.889	0.429	-7.477	1.00	23.81
15	HETATM	1935	C3	DES	A	600	9.814	0.804	-6.488	1.00	21.88
	HETATM	1936	O3	DES	A	600	11.125	0.901	-6.839	1.00	22.32
	HETATM	1937	C2	DES	A	600	9.423	1.066	-5.161	1.00	19.74
	HETATM	1938	C1	DES	A	600	8.066	0.937	-4.838	1.00	21.25
	HETATM	1939	C8	DES	A	600	4.894	1.765	-5.443	1.00	21.47
20	HETATM	1940	C9	DES	A	600	4.959	2.468	-4.070	1.00	21.38
	HETATM	1941	CL	CL	A	601	14.781	-3.035	-17.739	1.00	24.10
	ATOM	1942	CB	SER	B	305	12.321	21.086	25.295	1.00	64.27
	ATOM	1943	C	SER	B	305	12.672	22.102	27.548	1.00	64.37
	ATOM	1944	O	SER	B	305	13.701	22.760	27.702	1.00	66.90
25	ATOM	1945	N	SER	B	305	12.045	23.521	25.606	1.00	63.72
	ATOM	1946	CA	SER	B	305	11.875	22.187	26.251	1.00	64.21
	ATOM	1947	N	LEU	B	306	12.193	21.293	28.484	1.00	63.09
	ATOM	1948	CA	LEU	B	306	12.884	21.133	29.757	1.00	60.98
	ATOM	1949	CB	LEU	B	306	11.884	21.200	30.913	1.00	61.23
30	ATOM	1950	CG	LEU	B	306	12.221	20.417	32.183	1.00	62.23
	ATOM	1951	CD1	LEU	B	306	13.304	21.144	32.966	1.00	62.56
	ATOM	1952	CD2	LEU	B	306	10.965	20.258	33.027	1.00	64.31
	ATOM	1953	C	LEU	B	306	13.660	19.819	29.803	1.00	58.39
	ATOM	1954	O	LEU	B	306	14.570	19.654	30.614	1.00	58.56
35	ATOM	1955	N	ALA	B	307	13.293	18.881	28.933	1.00	54.82
	ATOM	1956	CA	ALA	B	307	13.971	17.589	28.861	1.00	50.62
	ATOM	1957	CB	ALA	B	307	13.092	16.584	28.143	1.00	51.30
	ATOM	1958	C	ALA	B	307	15.303	17.719	28.122	1.00	46.84
	ATOM	1959	O	ALA	B	307	16.196	16.885	28.274	1.00	45.62
40	ATOM	1960	N	LEU	B	308	15.431	18.769	27.320	1.00	43.46
	ATOM	1961	CA	LEU	B	308	16.643	18.983	26.542	1.00	43.01
	ATOM	1962	CB	LEU	B	308	16.413	20.100	25.526	1.00	41.32
	ATOM	1963	CG	LEU	B	308	16.315	19.708	24.051	1.00	43.10
	ATOM	1964	CD1	LEU	B	308	15.942	18.239	23.903	1.00	40.51
45	ATOM	1965	CD2	LEU	B	308	15.287	20.602	23.375	1.00	39.80
	ATOM	1966	C	LEU	B	308	17.874	19.297	27.385	1.00	42.11
	ATOM	1967	O	LEU	B	308	19.000	19.102	26.932	1.00	44.34
	ATOM	1968	N	SER	B	309	17.669	19.775	28.608	1.00	40.88
	ATOM	1969	CA	SER	B	309	18.796	20.100	29.475	1.00	42.79
50	ATOM	1970	CB	SER	B	309	18.562	21.447	30.163	1.00	41.25
	ATOM	1971	OG	SER	B	309	17.459	21.379	31.046	1.00	46.67
	ATOM	1972	C	SER	B	309	19.072	19.028	30.529	1.00	42.60
	ATOM	1973	O	SER	B	309	20.053	19.119	31.269	1.00	44.18
	ATOM	1974	N	LEU	B	310	18.217	18.012	30.596	1.00	39.44
55	ATOM	1975	CA	LEU	B	310	18.394	16.936	31.569	1.00	37.62
	ATOM	1976	CB	LEU	B	310	17.205	15.969	31.499	1.00	38.84
	ATOM	1977	CG	LEU	B	310	16.216	15.873	32.668	1.00	42.43
	ATOM	1978	CD1	LEU	B	310	16.040	17.219	33.355	1.00	42.55
	ATOM	1979	CD2	LEU	B	310	14.881	15.380	32.138	1.00	39.69
60	ATOM	1980	C	LEU	B	310	19.691	16.174	31.285	1.00	34.11
	ATOM	1981	O	LEU	B	310	20.111	16.070	30.139	1.00	34.41

5	ATOM	1982	N	THR	B	311	20.339	15.662	32.326	1.00	34.04
	ATOM	1983	CA	THR	B	311	21.564	14.888	32.127	1.00	32.34
	ATOM	1984	CB	THR	B	311	22.434	14.824	33.399	1.00	31.75
	ATOM	1985	OG1	THR	B	311	21.724	14.116	34.420	1.00	36.20
10	ATOM	1986	CG2	THR	B	311	22.782	16.212	33.893	1.00	31.05
	ATOM	1987	C	THR	B	311	21.145	13.460	31.790	1.00	32.37
	ATOM	1988	O	THR	B	311	19.967	13.117	31.899	1.00	28.16
	ATOM	1989	N	ALA	B	312	22.106	12.628	31.396	1.00	33.23
15	ATOM	1990	CA	ALA	B	312	21.811	11.237	31.053	1.00	35.63
	ATOM	1991	CB	ALA	B	312	23.077	10.527	30.577	1.00	34.00
	ATOM	1992	C	ALA	B	312	21.210	10.489	32.240	1.00	34.29
	ATOM	1993	O	ALA	B	312	20.226	9.766	32.089	1.00	33.10
20	ATOM	1994	N	ASP	B	313	21.800	10.665	33.419	1.00	33.90
	ATOM	1995	CA	ASP	B	313	21.304	9.994	34.615	1.00	34.19
	ATOM	1996	CB	ASP	B	313	22.258	10.219	35.788	1.00	42.09
	ATOM	1997	CG	ASP	B	313	23.494	9.358	35.700	1.00	44.87
25	ATOM	1998	OD1	ASP	B	313	24.586	9.858	36.040	1.00	51.57
	ATOM	1999	OD2	ASP	B	313	23.377	8.184	35.290	1.00	46.79
	ATOM	2000	C	ASP	B	313	19.925	10.520	34.971	1.00	31.99
	ATOM	2001	O	ASP	B	313	19.056	9.768	35.426	1.00	32.03
30	ATOM	2002	N	GLN	B	314	19.733	11.819	34.763	1.00	29.38
	ATOM	2003	CA	GLN	B	314	18.458	12.457	35.046	1.00	29.73
	ATOM	2004	CB	GLN	B	314	18.562	13.966	34.832	1.00	32.88
	ATOM	2005	CG	GLN	B	314	18.970	14.732	36.085	1.00	36.47
35	ATOM	2006	CD	GLN	B	314	19.213	16.208	35.815	1.00	36.76
	ATOM	2007	OE1	GLN	B	314	19.300	16.634	34.664	1.00	38.79
	ATOM	2008	NE2	GLN	B	314	19.327	16.995	36.880	1.00	39.72
	ATOM	2009	C	GLN	B	314	17.409	11.873	34.116	1.00	29.11
40	ATOM	2010	O	GLN	B	314	16.274	11.620	34.522	1.00	28.82
	ATOM	2011	N	MET	B	315	17.801	11.657	32.864	1.00	27.27
	ATOM	2012	CA	MET	B	315	16.900	11.079	31.872	1.00	30.41
	ATOM	2013	CB	MET	B	315	17.595	11.029	30.509	1.00	30.10
45	ATOM	2014	CG	MET	B	315	16.787	10.345	29.421	1.00	38.02
	ATOM	2015	SD	MET	B	315	15.252	11.220	29.065	1.00	41.12
	ATOM	2016	CE	MET	B	315	15.890	12.835	28.611	1.00	39.32
	ATOM	2017	C	MET	B	315	16.490	9.665	32.311	1.00	27.99
50	ATOM	2018	O	MET	B	315	15.302	9.351	32.396	1.00	26.60
	ATOM	2019	N	VAL	B	316	17.481	8.823	32.598	1.00	27.26
	ATOM	2020	CA	VAL	B	316	17.229	7.447	33.027	1.00	24.54
	ATOM	2021	CB	VAL	B	316	18.554	6.708	33.351	1.00	26.22
55	ATOM	2022	CG1	VAL	B	316	18.272	5.404	34.096	1.00	29.81
	ATOM	2023	CG2	VAL	B	316	19.302	6.410	32.074	1.00	29.75
	ATOM	2024	C	VAL	B	316	16.326	7.389	34.258	1.00	27.22
	ATOM	2025	O	VAL	B	316	15.397	6.579	34.318	1.00	25.55
60	ATOM	2026	N	SER	B	317	16.601	8.243	35.242	1.00	24.40
	ATOM	2027	CA	SER	B	317	15.799	8.268	36.460	1.00	27.63
	ATOM	2028	CB	SER	B	317	16.358	9.294	37.451	1.00	31.68
	ATOM	2029	OG	SER	B	317	17.492	8.771	38.112	1.00	39.97
65	ATOM	2030	C	SER	B	317	14.346	8.600	36.154	1.00	26.73
	ATOM	2031	O	SER	B	317	13.434	7.932	36.648	1.00	25.65
	ATOM	2032	N	ALA	B	318	14.135	9.634	35.342	1.00	24.19
	ATOM	2033	CA	ALA	B	318	12.786	10.049	34.969	1.00	24.17
70	ATOM	2034	CB	ALA	B	318	12.850	11.250	34.022	1.00	21.44
	ATOM	2035	C	ALA	B	318	12.038	8.890	34.306	1.00	21.63
	ATOM	2036	O	ALA	B	318	10.902	8.598	34.648	1.00	20.25
	ATOM	2037	N	LEU	B	319	12.695	8.225	33.364	1.00	23.37
75	ATOM	2038	CA	LEU	B	319	12.098	7.102	32.652	1.00	25.42

5	ATOM	2039	CB	LEU	B	319	13.050	6.635	31.548	1.00	22.03
	ATOM	2040	CG	LEU	B	319	13.264	7.622	30.394	1.00	20.71
	ATOM	2041	CD1	LEU	B	319	14.146	6.995	29.331	1.00	23.60
	ATOM	2042	CD2	LEU	B	319	11.918	8.020	29.803	1.00	23.82
	ATOM	2043	C	LEU	B	319	11.729	5.926	33.564	1.00	27.26
10	ATOM	2044	O	LEU	B	319	10.615	5.396	33.488	1.00	28.91
	ATOM	2045	N	LEU	B	320	12.656	5.516	34.426	1.00	26.58
	ATOM	2046	CA	LEU	B	320	12.399	4.405	35.334	1.00	26.73
	ATOM	2047	CB	LEU	B	320	13.657	4.075	36.145	1.00	26.87
	ATOM	2048	CG	LEU	B	320	14.846	3.460	35.398	1.00	26.15
15	ATOM	2049	CD1	LEU	B	320	16.053	3.375	36.330	1.00	28.04
	ATOM	2050	CD2	LEU	B	320	14.484	2.076	34.895	1.00	26.96
	ATOM	2051	C	LEU	B	320	11.249	4.722	36.290	1.00	29.19
	ATOM	2052	O	LEU	B	320	10.449	3.849	36.631	1.00	26.66
	ATOM	2053	N	ASP	B	321	11.160	5.976	36.719	1.00	29.72
20	ATOM	2054	CA	ASP	B	321	10.112	6.371	37.647	1.00	31.36
	ATOM	2055	CB	ASP	B	321	10.494	7.683	38.336	1.00	36.60
	ATOM	2056	CG	ASP	B	321	11.407	7.461	39.535	1.00	46.11
	ATOM	2057	OD1	ASP	B	321	10.897	7.058	40.605	1.00	46.64
	ATOM	2058	OD2	ASP	B	321	12.635	7.676	39.402	1.00	45.98
25	ATOM	2059	C	ASP	B	321	8.742	6.494	36.989	1.00	28.29
	ATOM	2060	O	ASP	B	321	7.715	6.432	37.661	1.00	27.19
	ATOM	2061	N	ALA	B	322	8.726	6.650	35.672	1.00	28.34
	ATOM	2062	CA	ALA	B	322	7.469	6.779	34.950	1.00	25.55
	ATOM	2063	CB	ALA	B	322	7.668	7.668	33.728	1.00	24.11
30	ATOM	2064	C	ALA	B	322	6.911	5.420	34.523	1.00	22.80
	ATOM	2065	O	ALA	B	322	5.810	5.338	33.979	1.00	24.54
	ATOM	2066	N	GLU	B	323	7.662	4.355	34.781	1.00	20.16
	ATOM	2067	CA	GLU	B	323	7.229	3.021	34.386	1.00	21.44
	ATOM	2068	CB	GLU	B	323	8.196	1.982	34.938	1.00	23.72
35	ATOM	2069	CG	GLU	B	323	9.393	1.746	34.024	1.00	23.58
	ATOM	2070	CD	GLU	B	323	8.988	1.134	32.685	1.00	25.23
	ATOM	2071	OE1	GLU	B	323	8.852	1.881	31.692	1.00	21.74
	ATOM	2072	OE2	GLU	B	323	8.809	-0.095	32.624	1.00	25.49
	ATOM	2073	C	GLU	B	323	5.796	2.696	34.810	1.00	22.35
40	ATOM	2074	O	GLU	B	323	5.409	2.926	35.951	1.00	22.34
	ATOM	2075	N	PRO	B	324	4.986	2.165	33.880	1.00	19.10
	ATOM	2076	CD	PRO	B	324	5.286	1.806	32.483	1.00	19.11
	ATOM	2077	CA	PRO	B	324	3.607	1.839	34.242	1.00	22.04
	ATOM	2078	CB	PRO	B	324	2.919	1.658	32.893	1.00	21.96
45	ATOM	2079	CG	PRO	B	324	4.015	1.137	32.015	1.00	24.13
	ATOM	2080	C	PRO	B	324	3.619	0.556	35.060	1.00	23.44
	ATOM	2081	O	PRO	B	324	4.590	-0.200	35.028	1.00	22.20
	ATOM	2082	N	PRO	B	325	2.540	0.287	35.801	1.00	24.88
	ATOM	2083	CD	PRO	B	325	1.299	1.068	35.945	1.00	26.67
50	ATOM	2084	CA	PRO	B	325	2.520	-0.940	36.603	1.00	25.10
	ATOM	2085	CB	PRO	B	325	1.394	-0.691	37.595	1.00	27.09
	ATOM	2086	CG	PRO	B	325	0.448	0.205	36.854	1.00	26.87
	ATOM	2087	C	PRO	B	325	2.270	-2.192	35.776	1.00	25.77
	ATOM	2088	O	PRO	B	325	1.853	-2.118	34.617	1.00	21.69
55	ATOM	2089	N	ILE	B	326	2.538	-3.344	36.379	1.00	24.05
	ATOM	2090	CA	ILE	B	326	2.301	-4.620	35.722	1.00	22.51
	ATOM	2091	CB	ILE	B	326	3.303	-5.688	36.185	1.00	25.81
	ATOM	2092	CG2	ILE	B	326	3.011	-7.018	35.481	1.00	23.78
	ATOM	2093	CG1	ILE	B	326	4.729	-5.209	35.900	1.00	25.75
60	ATOM	2094	CD1	ILE	B	326	5.241	-5.585	34.533	1.00	27.78
	ATOM	2095	C	ILE	B	326	0.893	-5.020	36.149	1.00	23.63

5	ATOM	2096	O	ILE	B	326	0.632	-5.231	37.332	1.00	24.81
	ATOM	2097	N	LEU	B	327	-0.018	-5.104	35.188	1.00	19.44
	ATOM	2098	CA	LEU	B	327	-1.399	-5.437	35.493	1.00	17.03
	ATOM	2099	CB	LEU	B	327	-2.336	-4.747	34.493	1.00	18.39
10	ATOM	2100	CG	LEU	B	327	-2.201	-3.216	34.373	1.00	20.69
	ATOM	2101	CD1	LEU	B	327	-3.245	-2.679	33.406	1.00	14.87
	ATOM	2102	CD2	LEU	B	327	-2.384	-2.570	35.742	1.00	14.39
	ATOM	2103	C	LEU	B	327	-1.662	-6.928	35.499	1.00	19.87
15	ATOM	2104	O	LEU	B	327	-0.854	-7.722	35.014	1.00	20.90
	ATOM	2105	N	TYR	B	328	-2.803	-7.300	36.066	1.00	20.92
	ATOM	2106	CA	TYR	B	328	-3.202	-8.692	36.135	1.00	21.79
	ATOM	2107	CB	TYR	B	328	-3.658	-9.050	37.550	1.00	22.91
20	ATOM	2108	CG	TYR	B	328	-2.515	-9.376	38.468	1.00	24.60
	ATOM	2109	CD1	TYR	B	328	-2.118	-10.696	38.677	1.00	25.93
	ATOM	2110	CE1	TYR	B	328	-1.034	-11.000	39.498	1.00	28.10
	ATOM	2111	CD2	TYR	B	328	-1.802	-8.362	39.103	1.00	29.46
25	ATOM	2112	CE2	TYR	B	328	-0.716	-8.654	39.926	1.00	35.30
	ATOM	2113	CZ	TYR	B	328	-0.338	-9.973	40.117	1.00	32.59
	ATOM	2114	OH	TYR	B	328	0.739	-10.257	40.923	1.00	37.24
	ATOM	2115	C	TYR	B	328	-4.336	-8.944	35.168	1.00	22.25
30	ATOM	2116	O	TYR	B	328	-5.115	-8.039	34.849	1.00	19.77
	ATOM	2117	N	SER	B	329	-4.420	-10.180	34.698	1.00	25.81
	ATOM	2118	CA	SER	B	329	-5.480	-10.571	33.787	1.00	29.39
	ATOM	2119	CB	SER	B	329	-5.002	-11.710	32.887	1.00	27.65
35	ATOM	2120	OG	SER	B	329	-6.091	-12.329	32.233	1.00	28.98
	ATOM	2121	C	SER	B	329	-6.625	-11.042	34.673	1.00	33.17
	ATOM	2122	O	SER	B	329	-6.453	-11.157	35.888	1.00	32.52
	ATOM	2123	N	GLU	B	330	-7.792	-11.289	34.084	1.00	38.75
40	ATOM	2124	CA	GLU	B	330	-8.930	-11.776	34.859	1.00	44.91
	ATOM	2125	CB	GLU	B	330	-10.134	-11.999	33.951	1.00	45.63
	ATOM	2126	C	GLU	B	330	-8.493	-13.093	35.491	1.00	48.62
	ATOM	2127	O	GLU	B	330	-7.739	-13.851	34.882	1.00	52.37
45	ATOM	2128	N	TYR	B	331	-8.952	-13.366	36.707	1.00	51.75
	ATOM	2129	CA	TYR	B	331	-8.575	-14.596	37.396	1.00	55.25
	ATOM	2130	CB	TYR	B	331	-8.538	-14.365	38.911	1.00	53.04
	ATOM	2131	CG	TYR	B	331	-9.769	-13.668	39.440	1.00	50.70
50	ATOM	2132	CD1	TYR	B	331	-10.880	-14.400	39.856	1.00	47.09
	ATOM	2133	CE1	TYR	B	331	-12.035	-13.762	40.292	1.00	46.43
	ATOM	2134	CD2	TYR	B	331	-9.842	-12.273	39.478	1.00	47.52
	ATOM	2135	CE2	TYR	B	331	-10.993	-11.625	39.913	1.00	43.98
55	ATOM	2136	CZ	TYR	B	331	-12.086	-12.376	40.314	1.00	44.33
	ATOM	2137	OH	TYR	B	331	-13.239	-11.747	40.715	1.00	45.31
	ATOM	2138	C	TYR	B	331	-9.528	-15.743	37.075	1.00	60.11
	ATOM	2139	O	TYR	B	331	-10.748	-15.569	37.066	1.00	63.13
60	ATOM	2140	N	ASP	B	332	-8.952	-16.913	36.809	1.00	61.60
	ATOM	2141	CA	ASP	B	332	-9.704	-18.124	36.490	1.00	63.58
	ATOM	2142	CB	ASP	B	332	-10.637	-17.895	35.298	1.00	65.11
	ATOM	2143	CG	ASP	B	332	-11.723	-18.953	35.200	1.00	65.32
55	ATOM	2144	OD1	ASP	B	332	-11.420	-20.136	35.463	1.00	63.69
	ATOM	2145	OD2	ASP	B	332	-12.876	-18.602	34.866	1.00	63.61
	ATOM	2146	C	ASP	B	332	-8.707	-19.227	36.153	1.00	62.86
	ATOM	2147	O	ASP	B	332	-7.853	-19.056	35.287	1.00	62.26
60	ATOM	2148	N	PRO	B	333	-8.811	-20.379	36.833	1.00	63.96
	ATOM	2149	CD	PRO	B	333	-9.808	-20.690	37.875	1.00	64.24
	ATOM	2150	CA	PRO	B	333	-7.901	-21.503	36.596	1.00	64.24
	ATOM	2151	CB	PRO	B	333	-8.015	-22.325	37.874	1.00	64.70
60	ATOM	2152	CG	PRO	B	333	-9.410	-22.071	38.347	1.00	65.00



5	ATOM	2153	C	PRO	B	333	-8.180	-22.340	35.351	1.00	63.90
	ATOM	2154	O	PRO	B	333	-7.384	-23.214	35.007	1.00	63.70
	ATOM	2155	N	THR	B	334	-9.303	-22.084	34.683	1.00	63.83
	ATOM	2156	CA	THR	B	334	-9.649	-22.832	33.475	1.00	63.77
	ATOM	2157	CB	THR	B	334	-11.065	-22.477	32.975	1.00	64.63
10	ATOM	2158	OG1	THR	B	334	-11.132	-21.078	32.675	1.00	65.95
	ATOM	2159	CG2	THR	B	334	-12.102	-22.817	34.036	1.00	65.09
	ATOM	2160	C	THR	B	334	-8.634	-22.499	32.388	1.00	62.62
	ATOM	2161	O	THR	B	334	-8.931	-21.774	31.437	1.00	60.15
	ATOM	2162	N	ARG	B	335	-7.432	-23.043	32.553	1.00	63.14
15	ATOM	2163	CA	ARG	B	335	-6.324	-22.820	31.633	1.00	60.70
	ATOM	2164	CB	ARG	B	335	-5.130	-23.667	32.050	1.00	58.73
	ATOM	2165	C	ARG	B	335	-6.667	-23.086	30.174	1.00	59.71
	ATOM	2166	O	ARG	B	335	-6.302	-22.298	29.298	1.00	62.33
	ATOM	2167	N	PRO	B	336	-7.377	-24.194	29.884	1.00	55.25
20	ATOM	2168	CD	PRO	B	336	-7.938	-25.227	30.769	1.00	53.53
	ATOM	2169	CA	PRO	B	336	-7.698	-24.437	28.471	1.00	50.10
	ATOM	2170	CB	PRO	B	336	-8.399	-25.799	28.476	1.00	49.70
	ATOM	2171	CG	PRO	B	336	-8.164	-26.372	29.844	1.00	50.71
	ATOM	2172	C	PRO	B	336	-8.602	-23.324	27.954	1.00	44.54
25	ATOM	2173	O	PRO	B	336	-9.809	-23.342	28.179	1.00	44.14
	ATOM	2174	N	PHE	B	337	-8.007	-22.350	27.274	1.00	39.18
	ATOM	2175	CA	PHE	B	337	-8.764	-21.223	26.742	1.00	38.25
	ATOM	2176	CB	PHE	B	337	-7.850	-20.003	26.567	1.00	36.98
	ATOM	2177	CG	PHE	B	337	-7.229	-19.517	27.846	1.00	36.81
30	ATOM	2178	CD1	PHE	B	337	-5.846	-19.511	28.002	1.00	38.89
	ATOM	2179	CD2	PHE	B	337	-8.023	-19.062	28.893	1.00	35.97
	ATOM	2180	CE1	PHE	B	337	-5.262	-19.059	29.185	1.00	36.85
	ATOM	2181	CE2	PHE	B	337	-7.449	-18.608	30.079	1.00	37.15
	ATOM	2182	CZ	PHE	B	337	-6.064	-18.607	30.224	1.00	38.40
35	ATOM	2183	C	PHE	B	337	-9.420	-21.535	25.402	1.00	36.81
	ATOM	2184	O	PHE	B	337	-8.962	-22.399	24.658	1.00	36.26
	ATOM	2185	N	SER	B	338	-10.504	-20.828	25.107	1.00	35.85
	ATOM	2186	CA	SER	B	338	-11.198	-20.981	23.836	1.00	34.76
	ATOM	2187	CB	SER	B	338	-12.713	-20.948	24.035	1.00	34.85
40	ATOM	2188	OG	SER	B	338	-13.164	-19.621	24.235	1.00	33.53
	ATOM	2189	C	SER	B	338	-10.761	-19.761	23.037	1.00	34.99
	ATOM	2190	O	SER	B	338	-10.143	-18.855	23.591	1.00	34.32
	ATOM	2191	N	GLU	B	339	-11.075	-19.722	21.750	1.00	33.01
	ATOM	2192	CA	GLU	B	339	-10.682	-18.579	20.950	1.00	33.94
45	ATOM	2193	CB	GLU	B	339	-11.146	-18.737	19.501	1.00	33.79
	ATOM	2194	CG	GLU	B	339	-10.758	-17.553	18.623	1.00	39.11
	ATOM	2195	CD	GLU	B	339	-10.865	-17.852	17.137	1.00	43.17
	ATOM	2196	OE1	GLU	B	339	-11.990	-17.785	16.600	1.00	45.28
	ATOM	2197	OE2	GLU	B	339	-9.824	-18.152	16.510	1.00	39.19
50	ATOM	2198	C	GLU	B	339	-11.265	-17.295	21.531	1.00	34.28
	ATOM	2199	O	GLU	B	339	-10.575	-16.283	21.631	1.00	33.65
	ATOM	2200	N	ALA	B	340	-12.535	-17.339	21.920	1.00	31.12
	ATOM	2201	CA	ALA	B	340	-13.194	-16.164	22.469	1.00	29.10
	ATOM	2202	CB	ALA	B	340	-14.696	-16.412	22.573	1.00	33.84
55	ATOM	2203	C	ALA	B	340	-12.639	-15.731	23.826	1.00	28.98
	ATOM	2204	O	ALA	B	340	-12.431	-14.541	24.060	1.00	30.48
	ATOM	2205	N	SER	B	341	-12.407	-16.691	24.719	1.00	26.66
	ATOM	2206	CA	SER	B	341	-11.882	-16.386	26.044	1.00	24.26
	ATOM	2207	CB	SER	B	341	-11.867	-17.643	26.923	1.00	27.04
60	ATOM	2208	OG	SER	B	341	-10.851	-18.541	26.515	1.00	33.84
	ATOM	2209	C	SER	B	341	-10.479	-15.793	25.960	1.00	23.97

5	ATOM	2210	O	SER	B	341	-10.171	-14.824	26.651	1.00	21.56
	ATOM	2211	N	MET	B	342	-9.631	-16.368	25.114	1.00	26.83
	ATOM	2212	CA	MET	B	342	-8.271	-15.865	24.954	1.00	27.24
	ATOM	2213	CB	MET	B	342	-7.477	-16.758	24.001	1.00	30.45
	ATOM	2214	CG	MET	B	342	-6.038	-16.300	23.802	1.00	35.35
10	ATOM	2215	SD	MET	B	342	-4.866	-17.667	23.777	1.00	44.57
	ATOM	2216	CE	MET	B	342	-4.034	-17.341	22.244	1.00	41.37
	ATOM	2217	C	MET	B	342	-8.322	-14.448	24.385	1.00	25.31
	ATOM	2218	O	MET	B	342	-7.653	-13.541	24.874	1.00	26.67
	ATOM	2219	N	MET	B	343	-9.114	-14.278	23.345	1.00	25.75
15	ATOM	2220	CA	MET	B	343	-9.262	-12.979	22.712	1.00	25.47
	ATOM	2221	CB	MET	B	343	-10.210	-13.088	21.528	1.00	23.51
	ATOM	2222	CG	MET	B	343	-9.540	-13.618	20.273	1.00	28.86
	ATOM	2223	SD	MET	B	343	-8.325	-12.456	19.609	1.00	29.25
	ATOM	2224	CE	MET	B	343	-9.344	-11.015	19.371	1.00	28.74
20	ATOM	2225	C	MET	B	343	-9.798	-11.966	23.712	1.00	25.37
	ATOM	2226	O	MET	B	343	-9.360	-10.810	23.728	1.00	24.98
	ATOM	2227	N	GLY	B	344	-10.739	-12.403	24.536	1.00	23.91
	ATOM	2228	CA	GLY	B	344	-11.320	-11.526	25.536	1.00	22.43
	ATOM	2229	C	GLY	B	344	-10.313	-11.103	26.592	1.00	22.06
25	ATOM	2230	O	GLY	B	344	-10.262	-9.934	26.982	1.00	20.87
	ATOM	2231	N	LEU	B	345	-9.511	-12.048	27.063	1.00	19.36
	ATOM	2232	CA	LEU	B	345	-8.520	-11.748	28.083	1.00	25.74
	ATOM	2233	CB	LEU	B	345	-7.886	-13.040	28.600	1.00	26.78
	ATOM	2234	CG	LEU	B	345	-8.794	-14.010	29.362	1.00	30.04
30	ATOM	2235	CD1	LEU	B	345	-8.099	-15.357	29.488	1.00	28.39
	ATOM	2236	CD2	LEU	B	345	-9.122	-13.443	30.736	1.00	29.93
	ATOM	2237	C	LEU	B	345	-7.425	-10.822	27.550	1.00	23.24
	ATOM	2238	O	LEU	B	345	-7.037	-9.865	28.212	1.00	23.43
	ATOM	2239	N	LEU	B	346	-6.937	-11.108	26.350	1.00	21.92
35	ATOM	2240	CA	LEU	B	346	-5.874	-10.303	25.763	1.00	22.71
	ATOM	2241	CB	LEU	B	346	-5.343	-10.962	24.486	1.00	23.17
	ATOM	2242	CG	LEU	B	346	-4.684	-12.331	24.668	1.00	20.66
	ATOM	2243	CD1	LEU	B	346	-4.303	-12.916	23.309	1.00	18.75
	ATOM	2244	CD2	LEU	B	346	-3.464	-12.188	25.553	1.00	20.84
40	ATOM	2245	C	LEU	B	346	-6.304	-8.873	25.458	1.00	22.99
	ATOM	2246	O	LEU	B	346	-5.540	-7.935	25.695	1.00	22.07
	ATOM	2247	N	THR	B	347	-7.516	-8.699	24.937	1.00	20.53
	ATOM	2248	CA	THR	B	347	-7.987	-7.357	24.608	1.00	21.89
	ATOM	2249	CB	THR	B	347	-9.152	-7.388	23.601	1.00	21.65
45	ATOM	2250	OG1	THR	B	347	-10.218	-8.190	24.123	1.00	19.65
	ATOM	2251	CG2	THR	B	347	-8.676	-7.955	22.262	1.00	22.01
	ATOM	2252	C	THR	B	347	-8.426	-6.590	25.853	1.00	23.60
	ATOM	2253	O	THR	B	347	-8.358	-5.357	25.883	1.00	20.31
	ATOM	2254	N	ASN	B	348	-8.884	-7.314	26.874	1.00	22.27
50	ATOM	2255	CA	ASN	B	348	-9.293	-6.667	28.114	1.00	23.99
	ATOM	2256	CB	ASN	B	348	-10.008	-7.642	29.056	1.00	22.32
	ATOM	2257	CG	ASN	B	348	-10.342	-7.022	30.398	1.00	28.26
	ATOM	2258	OD1	ASN	B	348	-9.478	-6.746	31.216	1.00	27.14
	ATOM	2259	ND2	ASN	B	348	-11.647	-6.764	30.625	1.00	27.02
55	ATOM	2260	C	ASN	B	348	-8.035	-6.120	28.798	1.00	19.48
	ATOM	2261	O	ASN	B	348	-8.014	-4.991	29.271	1.00	18.26
	ATOM	2262	N	LEU	B	349	-6.984	-6.931	28.832	1.00	19.07
	ATOM	2263	CA	LEU	B	349	-5.724	-6.516	29.446	1.00	20.37
	ATOM	2264	CB	LEU	B	349	-4.716	-7.674	29.434	1.00	18.21
60	ATOM	2265	CG	LEU	B	349	-3.297	-7.316	29.889	1.00	18.24
	ATOM	2266	CD1	LEU	B	349	-3.323	-6.904	31.356	1.00	12.44

5	ATOM	2267	CD2	LEU	B	349	-2.370	-8.504	29.672	1.00	21.28
	ATOM	2268	C	LEU	B	349	-5.131	-5.307	28.718	1.00	19.92
	ATOM	2269	O	LEU	B	349	-4.738	-4.322	29.349	1.00	16.56
	ATOM	2270	N	ALA	B	350	-5.067	-5.391	27.391	1.00	16.67
	ATOM	2271	CA	ALA	B	350	-4.529	-4.308	26.578	1.00	17.11
10	ATOM	2272	CB	ALA	B	350	-4.587	-4.690	25.095	1.00	14.15
	ATOM	2273	C	ALA	B	350	-5.272	-2.988	26.805	1.00	17.92
	ATOM	2274	O	ALA	B	350	-4.650	-1.926	26.904	1.00	18.71
	ATOM	2275	N	ASP	B	351	-6.600	-3.053	26.857	1.00	17.51
	ATOM	2276	CA	ASP	B	351	-7.409	-1.856	27.074	1.00	16.57
15	ATOM	2277	CB	ASP	B	351	-8.902	-2.202	27.041	1.00	18.97
	ATOM	2278	CG	ASP	B	351	-9.785	-0.974	26.858	1.00	21.80
	ATOM	2279	OD1	ASP	B	351	-9.660	-0.292	25.824	1.00	24.62
	ATOM	2280	OD2	ASP	B	351	-10.604	-0.682	27.754	1.00	22.78
	ATOM	2281	C	ASP	B	351	-7.064	-1.228	28.415	1.00	16.81
20	ATOM	2282	O	ASP	B	351	-6.963	-0.009	28.534	1.00	15.75
	ATOM	2283	N	ARG	B	352	-6.894	-2.056	29.438	1.00	13.97
	ATOM	2284	CA	ARG	B	352	-6.552	-1.509	30.742	1.00	16.09
	ATOM	2285	CB	ARG	B	352	-6.728	-2.571	31.833	1.00	15.78
	ATOM	2286	CG	ARG	B	352	-8.189	-2.819	32.189	1.00	17.93
25	ATOM	2287	CD	ARG	B	352	-8.323	-3.882	33.279	1.00	19.84
	ATOM	2288	NE	ARG	B	352	-8.010	-5.222	32.785	1.00	21.36
	ATOM	2289	CZ	ARG	B	352	-7.187	-6.075	33.387	1.00	21.18
	ATOM	2290	NH1	ARG	B	352	-6.579	-5.741	34.516	1.00	20.51
	ATOM	2291	NH2	ARG	B	352	-6.980	-7.275	32.864	1.00	28.51
30	ATOM	2292	C	ARG	B	352	-5.123	-0.975	30.728	1.00	15.81
	ATOM	2293	O	ARG	B	352	-4.835	0.057	31.339	1.00	15.61
	ATOM	2294	N	GLU	B	353	-4.231	-1.665	30.019	1.00	15.45
	ATOM	2295	CA	GLU	B	353	-2.838	-1.228	29.935	1.00	16.59
	ATOM	2296	CB	GLU	B	353	-1.990	-2.243	29.168	1.00	14.64
35	ATOM	2297	CG	GLU	B	353	-1.554	-3.456	29.973	1.00	18.23
	ATOM	2298	CD	GLU	B	353	-0.620	-4.355	29.176	1.00	22.72
	ATOM	2299	OE1	GLU	B	353	-1.099	-5.078	28.275	1.00	21.94
	ATOM	2300	OE2	GLU	B	353	0.599	-4.324	29.442	1.00	24.41
	ATOM	2301	C	GLU	B	353	-2.729	0.119	29.219	1.00	15.85
40	ATOM	2302	O	GLU	B	353	-1.872	0.939	29.540	1.00	13.76
	ATOM	2303	N	LEU	B	354	-3.594	0.335	28.235	1.00	12.93
	ATOM	2304	CA	LEU	B	354	-3.556	1.575	27.472	1.00	15.33
	ATOM	2305	CB	LEU	B	354	-4.616	1.534	26.360	1.00	16.44
	ATOM	2306	CG	LEU	B	354	-4.174	0.750	25.112	1.00	17.03
45	ATOM	2307	CD1	LEU	B	354	-5.373	0.509	24.189	1.00	16.70
	ATOM	2308	CD2	LEU	B	354	-3.069	1.531	24.384	1.00	14.52
	ATOM	2309	C	LEU	B	354	-3.747	2.805	28.361	1.00	12.78
	ATOM	2310	O	LEU	B	354	-3.123	3.850	28.141	1.00	14.28
	ATOM	2311	N	VAL	B	355	-4.600	2.682	29.369	1.00	12.60
50	ATOM	2312	CA	VAL	B	355	-4.844	3.791	30.279	1.00	16.78
	ATOM	2313	CB	VAL	B	355	-5.925	3.429	31.327	1.00	16.84
	ATOM	2314	CG1	VAL	B	355	-6.070	4.561	32.344	1.00	19.88
	ATOM	2315	CG2	VAL	B	355	-7.254	3.187	30.639	1.00	19.33
	ATOM	2316	C	VAL	B	355	-3.533	4.161	30.986	1.00	19.17
55	ATOM	2317	O	VAL	B	355	-3.158	5.328	31.049	1.00	17.30
	ATOM	2318	N	HIS	B	356	-2.826	3.160	31.499	1.00	19.68
	ATOM	2319	CA	HIS	B	356	-1.559	3.418	32.177	1.00	20.64
	ATOM	2320	CB	HIS	B	356	-1.110	2.174	32.945	1.00	21.03
	ATOM	2321	CG	HIS	B	356	-2.018	1.818	34.085	1.00	22.88
60	ATOM	2322	CD2	HIS	B	356	-3.128	1.045	34.135	1.00	21.70
	ATOM	2323	ND1	HIS	B	356	-1.838	2.312	35.358	1.00	19.24

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5	ATOM	2381	CA	ARG	B	363	5.996	11.414	32.109	1.00	27.74
	ATOM	2382	CB	ARG	B	363	5.887	10.457	33.298	1.00	28.93
	ATOM	2383	CG	ARG	B	363	4.650	10.704	34.158	1.00	36.07
	ATOM	2384	CD	ARG	B	363	4.569	9.745	35.344	1.00	42.83
	ATOM	2385	NE	ARG	B	363	4.477	8.344	34.928	1.00	49.79
10	ATOM	2386	CZ	ARG	B	363	3.395	7.582	35.080	1.00	51.48
	ATOM	2387	NH1	ARG	B	363	2.300	8.081	35.648	1.00	52.17
	ATOM	2388	NH2	ARG	B	363	3.405	6.316	34.668	1.00	40.24
	ATOM	2389	C	ARG	B	363	7.308	11.190	31.367	1.00	25.80
	ATOM	2390	O	ARG	B	363	8.374	11.183	31.975	1.00	29.36
15	ATOM	2391	N	VAL	B	364	7.231	11.009	30.053	1.00	24.28
	ATOM	2392	CA	VAL	B	364	8.431	10.823	29.248	1.00	21.87
	ATOM	2393	CB	VAL	B	364	8.116	10.048	27.947	1.00	21.84
	ATOM	2394	CG1	VAL	B	364	9.267	10.184	26.968	1.00	15.85
	ATOM	2395	CG2	VAL	B	364	7.860	8.560	28.268	1.00	16.24
20	ATOM	2396	C	VAL	B	364	8.925	12.241	28.923	1.00	28.14
	ATOM	2397	O	VAL	B	364	8.219	13.023	28.285	1.00	24.24
	ATOM	2398	N	PRO	B	365	10.141	12.591	29.375	1.00	28.57
	ATOM	2399	CD	PRO	B	365	11.061	11.726	30.137	1.00	30.58
	ATOM	2400	CA	PRO	B	365	10.719	13.919	29.138	1.00	32.16
25	ATOM	2401	CB	PRO	B	365	12.189	13.739	29.507	1.00	32.70
	ATOM	2402	CG	PRO	B	365	12.170	12.671	30.545	1.00	33.35
	ATOM	2403	C	PRO	B	365	10.546	14.464	27.726	1.00	32.22
	ATOM	2404	O	PRO	B	365	11.056	13.897	26.766	1.00	37.04
	ATOM	2405	N	GLY	B	366	9.821	15.570	27.609	1.00	34.09
30	ATOM	2406	CA	GLY	B	366	9.612	16.182	26.310	1.00	32.54
	ATOM	2407	C	GLY	B	366	8.241	15.969	25.700	1.00	33.46
	ATOM	2408	O	GLY	B	366	7.791	16.779	24.886	1.00	33.73
	ATOM	2409	N	PHE	B	367	7.564	14.895	26.096	1.00	31.08
	ATOM	2410	CA	PHE	B	367	6.250	14.593	25.542	1.00	28.60
35	ATOM	2411	CB	PHE	B	367	5.745	13.244	26.058	1.00	25.96
	ATOM	2412	CG	PHE	B	367	4.629	12.671	25.239	1.00	22.75
	ATOM	2413	CD1	PHE	B	367	3.313	12.771	25.669	1.00	22.62
	ATOM	2414	CD2	PHE	B	367	4.897	12.025	24.033	1.00	22.29
	ATOM	2415	CE1	PHE	B	367	2.272	12.233	24.914	1.00	25.63
40	ATOM	2416	CE2	PHE	B	367	3.867	11.486	23.272	1.00	20.82
	ATOM	2417	CZ	PHE	B	367	2.553	11.588	23.711	1.00	25.50
	ATOM	2418	C	PHE	B	367	5.178	15.646	25.781	1.00	26.79
	ATOM	2419	O	PHE	B	367	4.458	16.001	24.854	1.00	23.37
	ATOM	2420	N	VAL	B	368	5.049	16.143	27.009	1.00	31.26
45	ATOM	2421	CA	VAL	B	368	4.020	17.151	27.277	1.00	35.71
	ATOM	2422	CB	VAL	B	368	3.817	17.412	28.795	1.00	35.98
	ATOM	2423	CG1	VAL	B	368	2.944	16.320	29.392	1.00	37.64
	ATOM	2424	CG2	VAL	B	368	5.157	17.495	29.508	1.00	35.81
	ATOM	2425	C	VAL	B	368	4.328	18.482	26.598	1.00	35.87
50	ATOM	2426	O	VAL	B	368	3.450	19.330	26.457	1.00	37.71
	ATOM	2427	N	ASP	B	369	5.572	18.665	26.175	1.00	35.49
	ATOM	2428	CA	ASP	B	369	5.950	19.904	25.503	1.00	36.54
	ATOM	2429	CB	ASP	B	369	7.466	19.963	25.309	1.00	39.79
	ATOM	2430	CG	ASP	B	369	8.213	20.169	26.615	1.00	44.33
55	ATOM	2431	OD1	ASP	B	369	9.409	19.807	26.684	1.00	48.45
	ATOM	2432	OD2	ASP	B	369	7.604	20.693	27.572	1.00	43.27
	ATOM	2433	C	ASP	B	369	5.248	19.997	24.149	1.00	34.49
	ATOM	2434	O	ASP	B	369	5.131	21.074	23.571	1.00	34.51
	ATOM	2435	N	LEU	B	370	4.776	18.859	23.653	1.00	30.97
60	ATOM	2436	CA	LEU	B	370	4.086	18.809	22.370	1.00	29.80
	ATOM	2437	CB	LEU	B	370	4.145	17.389	21.799	1.00	27.27

5	ATOM	2438	CG	LEU	B	370	5.522	16.733	21.688	1.00	28.07
	ATOM	2439	CD1	LEU	B	370	5.353	15.242	21.400	1.00	30.38
	ATOM	2440	CD2	LEU	B	370	6.316	17.396	20.574	1.00	22.82
	ATOM	2441	C	LEU	B	370	2.628	19.218	22.521	1.00	28.04
	ATOM	2442	O	LEU	B	370	2.066	19.151	23.611	1.00	29.71
	ATOM	2443	N	THR	B	371	2.011	19.645	21.425	1.00	28.70
10	ATOM	2444	CA	THR	B	371	0.602	20.014	21.474	1.00	30.31
	ATOM	2445	CB	THR	B	371	0.150	20.690	20.163	1.00	31.96
	ATOM	2446	OG1	THR	B	371	0.284	19.763	19.080	1.00	29.49
	ATOM	2447	CG2	THR	B	371	0.991	21.930	19.878	1.00	29.98
	ATOM	2448	C	THR	B	371	-0.208	18.726	21.666	1.00	30.59
	ATOM	2449	O	THR	B	371	0.300	17.624	21.431	1.00	27.10
15	ATOM	2450	N	LEU	B	372	-1.461	18.863	22.087	1.00	27.65
	ATOM	2451	CA	LEU	B	372	-2.323	17.702	22.303	1.00	30.86
	ATOM	2452	CB	LEU	B	372	-3.722	18.147	22.737	1.00	30.11
	ATOM	2453	CG	LEU	B	372	-4.715	17.006	22.960	1.00	32.80
	ATOM	2454	CD1	LEU	B	372	-4.231	16.147	24.126	1.00	34.10
	ATOM	2455	CD2	LEU	B	372	-6.105	17.562	23.246	1.00	31.16
20	ATOM	2456	C	LEU	B	372	-2.437	16.863	21.034	1.00	31.77
	ATOM	2457	O	LEU	B	372	-2.417	15.629	21.078	1.00	27.06
	ATOM	2458	N	HIS	B	373	-2.564	17.548	19.905	1.00	31.30
25	ATOM	2459	CA	HIS	B	373	-2.685	16.888	18.614	1.00	31.35
	ATOM	2460	CB	HIS	B	373	-2.844	17.935	17.503	1.00	34.30
	ATOM	2461	CG	HIS	B	373	-2.503	17.430	16.132	1.00	41.27
	ATOM	2462	CD2	HIS	B	373	-3.293	17.105	15.079	1.00	42.50
	ATOM	2463	ND1	HIS	B	373	-1.205	17.220	15.715	1.00	43.69
	ATOM	2464	CE1	HIS	B	373	-1.210	16.787	14.465	1.00	48.87
30	ATOM	2465	NE2	HIS	B	373	-2.465	16.708	14.056	1.00	43.72
	ATOM	2466	C	HIS	B	373	-1.468	16.012	18.337	1.00	28.29
	ATOM	2467	O	HIS	B	373	-1.610	14.878	17.897	1.00	30.21
35	ATOM	2468	N	ASP	B	374	-0.275	16.541	18.589	1.00	28.85
	ATOM	2469	CA	ASP	B	374	0.950	15.783	18.350	1.00	28.28
	ATOM	2470	CB	ASP	B	374	2.178	16.678	18.535	1.00	31.33
	ATOM	2471	CG	ASP	B	374	2.433	17.577	17.333	1.00	39.07
	ATOM	2472	OD1	ASP	B	374	3.195	18.557	17.478	1.00	40.60
	ATOM	2473	OD2	ASP	B	374	1.874	17.305	16.246	1.00	38.64
40	ATOM	2474	C	ASP	B	374	1.029	14.592	19.303	1.00	29.05
	ATOM	2475	O	ASP	B	374	1.432	13.494	18.908	1.00	24.26
	ATOM	2476	N	GLN	B	375	0.642	14.814	20.556	1.00	24.52
45	ATOM	2477	CA	GLN	B	375	0.667	13.749	21.547	1.00	27.37
	ATOM	2478	CB	GLN	B	375	0.213	14.270	22.901	1.00	26.66
	ATOM	2479	CG	GLN	B	375	1.164	15.236	23.563	1.00	29.74
	ATOM	2480	CD	GLN	B	375	0.623	15.691	24.890	1.00	33.13
	ATOM	2481	OE1	GLN	B	375	-0.044	14.953	25.602	1.00	32.82
	ATOM	2482	NE2	GLN	B	375	0.895	16.953	25.236	1.00	33.98
50	ATOM	2483	C	GLN	B	375	-0.259	12.630	21.104	1.00	24.52
	ATOM	2484	O	GLN	B	375	0.074	11.451	21.221	1.00	23.56
	ATOM	2485	N	VAL	B	376	-1.426	13.013	20.599	1.00	21.87
	ATOM	2486	CA	VAL	B	376	-2.409	12.055	20.140	1.00	23.44
	ATOM	2487	CB	VAL	B	376	-3.718	12.760	19.717	1.00	22.09
	ATOM	2488	CG1	VAL	B	376	-4.572	11.823	18.877	1.00	24.14
55	ATOM	2489	CG2	VAL	B	376	-4.486	13.192	20.954	1.00	16.96
	ATOM	2490	C	VAL	B	376	-1.852	11.257	18.965	1.00	24.15
	ATOM	2491	O	VAL	B	376	-1.949	10.032	18.938	1.00	22.26
	ATOM	2492	N	HIS	B	377	-1.251	11.953	18.007	1.00	25.85
	ATOM	2493	CA	HIS	B	377	-0.689	11.284	16.843	1.00	25.68
	ATOM	2494	CB	HIS	B	377	-0.078	12.306	15.886	1.00	25.27

5	ATOM	2495	CG	HIS	B	377	0.535	11.690	14.667	1.00	30.63
	ATOM	2496	CD2	HIS	B	377	1.828	11.559	14.287	1.00	31.03
	ATOM	2497	ND1	HIS	B	377	-0.217	11.086	13.683	1.00	35.05
	ATOM	2498	CE1	HIS	B	377	0.588	10.607	12.750	1.00	33.12
	ATOM	2499	NE2	HIS	B	377	1.833	10.882	13.093	1.00	31.06
10	ATOM	2500	C	HIS	B	377	0.365	10.237	17.210	1.00	24.37
	ATOM	2501	O	HIS	B	377	0.321	9.109	16.719	1.00	21.47
	ATOM	2502	N	LEU	B	378	1.307	10.609	18.072	1.00	19.24
	ATOM	2503	CA	LEU	B	378	2.365	9.691	18.474	1.00	20.09
	ATOM	2504	CB	LEU	B	378	3.363	10.402	19.388	1.00	18.64
15	ATOM	2505	CG	LEU	B	378	4.230	11.489	18.736	1.00	22.15
	ATOM	2506	CD1	LEU	B	378	5.104	12.148	19.796	1.00	22.51
	ATOM	2507	CD2	LEU	B	378	5.094	10.885	17.638	1.00	20.68
	ATOM	2508	C	LEU	B	378	1.832	8.433	19.161	1.00	18.91
	ATOM	2509	O	LEU	B	378	2.262	7.320	18.859	1.00	17.52
20	ATOM	2510	N	LEU	B	379	0.888	8.610	20.077	1.00	18.25
	ATOM	2511	CA	LEU	B	379	0.317	7.486	20.795	1.00	18.60
	ATOM	2512	CB	LEU	B	379	-0.526	7.989	21.968	1.00	16.77
	ATOM	2513	CG	LEU	B	379	0.292	8.353	23.214	1.00	17.90
	ATOM	2514	CD1	LEU	B	379	-0.578	9.092	24.211	1.00	15.84
25	ATOM	2515	CD2	LEU	B	379	0.851	7.075	23.842	1.00	22.09
	ATOM	2516	C	LEU	B	379	-0.518	6.605	19.872	1.00	20.17
	ATOM	2517	O	LEU	B	379	-0.476	5.377	19.968	1.00	18.11
	ATOM	2518	N	GLU	B	380	-1.273	7.222	18.971	1.00	19.40
	ATOM	2519	CA	GLU	B	380	-2.086	6.435	18.049	1.00	20.19
30	ATOM	2520	CB	GLU	B	380	-2.994	7.350	17.222	1.00	22.43
	ATOM	2521	CG	GLU	B	380	-4.182	7.874	18.007	1.00	25.30
	ATOM	2522	CD	GLU	B	380	-5.070	8.789	17.188	1.00	29.44
	ATOM	2523	OE1	GLU	B	380	-6.206	9.066	17.625	1.00	31.70
	ATOM	2524	OE2	GLU	B	380	-4.631	9.230	16.110	1.00	31.75
35	ATOM	2525	C	GLU	B	380	-1.210	5.594	17.117	1.00	18.92
	ATOM	2526	O	GLU	B	380	-1.586	4.491	16.722	1.00	19.83
	ATOM	2527	N	ACYS	B	381	-0.039	6.113	16.772	0.75	17.41
	ATOM	2528	N	BCYS	B	381	-0.035	6.113	16.779	0.25	17.76
	ATOM	2529	CA	ACYS	B	381	0.860	5.384	15.887	0.75	20.19
40	ATOM	2530	CA	BCYS	B	381	0.875	5.407	15.884	0.25	17.50
	ATOM	2531	CB	ACYS	B	381	1.870	6.342	15.248	0.75	24.20
	ATOM	2532	CB	BCYS	B	381	1.830	6.406	15.226	0.25	16.63
	ATOM	2533	SG	ACYS	B	381	1.167	7.518	14.060	0.75	33.54
	ATOM	2534	SG	BCYS	B	381	3.048	5.656	14.128	0.25	10.36
45	ATOM	2535	C	ACYS	B	381	1.626	4.269	16.592	0.75	20.59
	ATOM	2536	C	BCYS	B	381	1.689	4.305	16.561	0.25	19.19
	ATOM	2537	O	ACYS	B	381	1.737	3.161	16.069	0.75	19.16
	ATOM	2538	O	BCYS	B	381	1.904	3.241	15.982	0.25	19.25
	ATOM	2539	N	ALA	B	382	2.134	4.560	17.785	1.00	19.04
50	ATOM	2540	CA	ALA	B	382	2.955	3.602	18.530	1.00	20.27
	ATOM	2541	CB	ALA	B	382	4.135	4.364	19.143	1.00	18.68
	ATOM	2542	C	ALA	B	382	2.356	2.702	19.607	1.00	16.82
	ATOM	2543	O	ALA	B	382	3.070	1.852	20.142	1.00	13.37
	ATOM	2544	N	TRP	B	383	1.074	2.855	19.916	1.00	15.30
55	ATOM	2545	CA	TRP	B	383	0.487	2.089	21.013	1.00	15.80
	ATOM	2546	CB	TRP	B	383	-1.009	2.410	21.160	1.00	16.63
	ATOM	2547	CG	TRP	B	383	-1.871	1.775	20.129	1.00	19.93
	ATOM	2548	CD2	TRP	B	383	-2.493	0.483	20.198	1.00	20.80
	ATOM	2549	CE2	TRP	B	383	-3.226	0.309	19.003	1.00	19.27
60	ATOM	2550	CE3	TRP	B	383	-2.506	-0.542	21.155	1.00	21.32
	ATOM	2551	CD1	TRP	B	383	-2.236	2.312	18.933	1.00	18.59

5	ATOM	2552	NE1	TRP	B	383	-3.051	1.439	18.250	1.00	23.67
	ATOM	2553	CZ2	TRP	B	383	-3.963	-0.853	18.733	1.00	21.55
	ATOM	2554	CZ3	TRP	B	383	-3.243	-1.702	20.888	1.00	20.29
	ATOM	2555	CH2	TRP	B	383	-3.960	-1.844	19.686	1.00	19.03
	ATOM	2556	C	TRP	B	383	0.701	0.579	21.020	1.00	17.35
10	ATOM	2557	O	TRP	B	383	0.982	0.010	22.077	1.00	13.92
	ATOM	2558	N	LEU	B	384	0.568	-0.087	19.879	1.00	14.07
	ATOM	2559	CA	LEU	B	384	0.773	-1.532	19.903	1.00	15.98
	ATOM	2560	CB	LEU	B	384	0.181	-2.200	18.656	1.00	12.19
	ATOM	2561	CG	LEU	B	384	0.173	-3.735	18.720	1.00	12.97
15	ATOM	2562	CD1	LEU	B	384	-0.352	-4.240	20.089	1.00	10.65
	ATOM	2563	CD2	LEU	B	384	-0.707	-4.259	17.586	1.00	17.84
	ATOM	2564	C	LEU	B	384	2.262	-1.861	20.034	1.00	14.64
	ATOM	2565	O	LEU	B	384	2.627	-2.833	20.690	1.00	13.78
	ATOM	2566	N	GLU	B	385	3.116	-1.046	19.414	1.00	14.96
20	ATOM	2567	CA	GLU	B	385	4.565	-1.260	19.509	1.00	13.79
	ATOM	2568	CB	GLU	B	385	5.336	-0.179	18.739	1.00	15.34
	ATOM	2569	CG	GLU	B	385	5.297	-0.312	17.207	1.00	15.38
	ATOM	2570	CD	GLU	B	385	6.162	0.738	16.520	1.00	23.97
	ATOM	2571	OE1	GLU	B	385	7.381	0.500	16.358	1.00	21.03
25	ATOM	2572	OE2	GLU	B	385	5.622	1.808	16.149	1.00	22.19
	ATOM	2573	C	GLU	B	385	4.963	-1.161	20.987	1.00	15.79
	ATOM	2574	O	GLU	B	385	5.788	-1.942	21.463	1.00	15.04
	ATOM	2575	N	ILE	B	386	4.389	-0.213	21.690	1.00	13.32
	ATOM	2576	CA	ILE	B	386	4.723	-0.019	23.108	1.00	14.06
30	ATOM	2577	CB	ILE	B	386	4.173	1.326	23.614	1.00	15.36
	ATOM	2578	CG2	ILE	B	386	4.374	1.451	25.130	1.00	15.97
	ATOM	2579	CG1	ILE	B	386	4.910	2.476	22.907	1.00	17.95
	ATOM	2580	CD1	ILE	B	386	4.118	3.768	22.874	1.00	21.12
	ATOM	2581	C	ILE	B	386	4.227	-1.164	23.993	1.00	14.97
35	ATOM	2582	O	ILE	B	386	4.905	-1.560	24.941	1.00	19.60
	ATOM	2583	N	LEU	B	387	3.038	-1.675	23.709	1.00	15.18
	ATOM	2584	CA	LEU	B	387	2.516	-2.791	24.478	1.00	15.98
	ATOM	2585	CB	LEU	B	387	1.070	-3.097	24.080	1.00	17.15
	ATOM	2586	CG	LEU	B	387	-0.031	-2.113	24.486	1.00	19.65
40	ATOM	2587	CD1	LEU	B	387	-1.371	-2.628	23.972	1.00	17.77
	ATOM	2588	CD2	LEU	B	387	-0.075	-1.966	26.002	1.00	15.38
	ATOM	2589	C	LEU	B	387	3.391	-4.013	24.180	1.00	14.69
	ATOM	2590	O	LEU	B	387	3.712	-4.792	25.076	1.00	14.03
	ATOM	2591	N	MET	B	388	3.785	-4.178	22.921	1.00	16.43
45	ATOM	2592	CA	MET	B	388	4.602	-5.329	22.547	1.00	16.67
	ATOM	2593	CB	MET	B	388	4.673	-5.460	21.026	1.00	14.83
	ATOM	2594	CG	MET	B	388	3.403	-6.066	20.453	1.00	13.91
	ATOM	2595	SD	MET	B	388	3.364	-6.193	18.675	1.00	17.23
	ATOM	2596	CE	MET	B	388	1.906	-7.225	18.511	1.00	14.97
50	ATOM	2597	C	MET	B	388	6.004	-5.332	23.133	1.00	20.19
	ATOM	2598	O	MET	B	388	6.460	-6.366	23.636	1.00	21.50
	ATOM	2599	N	ILE	B	389	6.707	-4.203	23.074	1.00	15.34
	ATOM	2600	CA	ILE	B	389	8.044	-4.209	23.634	1.00	15.59
	ATOM	2601	CB	ILE	B	389	8.836	-2.911	23.322	1.00	14.95
55	ATOM	2602	CG2	ILE	B	389	8.330	-1.746	24.158	1.00	12.81
	ATOM	2603	CG1	ILE	B	389	10.325	-3.164	23.602	1.00	17.24
	ATOM	2604	CD1	ILE	B	389	11.228	-1.972	23.357	1.00	15.65
	ATOM	2605	C	ILE	B	389	7.950	-4.446	25.147	1.00	14.30
	ATOM	2606	O	ILE	B	389	8.844	-5.044	25.739	1.00	18.72
60	ATOM	2607	N	GLY	B	390	6.855	-4.007	25.761	1.00	13.99
	ATOM	2608	CA	GLY	B	390	6.681	-4.219	27.189	1.00	14.87



5	ATOM	2609	C	GLY	B	390	6.444	-5.702	27.463	1.00	18.54
	ATOM	2610	O	GLY	B	390	6.989	-6.282	28.403	1.00	16.54
	ATOM	2611	N	LEU	B	391	5.623	-6.325	26.628	1.00	16.15
	ATOM	2612	CA	LEU	B	391	5.334	-7.743	26.775	1.00	18.91
	ATOM	2613	CB	LEU	B	391	4.332	-8.179	25.699	1.00	19.55
10	ATOM	2614	CG	LEU	B	391	4.157	-9.689	25.457	1.00	20.91
	ATOM	2615	CD1	LEU	B	391	3.580	-10.351	26.699	1.00	19.41
	ATOM	2616	CD2	LEU	B	391	3.232	-9.913	24.268	1.00	20.70
	ATOM	2617	C	LEU	B	391	6.649	-8.518	26.625	1.00	20.31
	ATOM	2618	O	LEU	B	391	7.002	-9.352	27.465	1.00	18.66
15	ATOM	2619	N	VAL	B	392	7.378	-8.215	25.557	1.00	18.71
	ATOM	2620	CA	VAL	B	392	8.649	-8.868	25.278	1.00	19.51
	ATOM	2621	CB	VAL	B	392	9.288	-8.281	24.005	1.00	23.77
	ATOM	2622	CG1	VAL	B	392	10.751	-8.687	23.920	1.00	24.63
	ATOM	2623	CG2	VAL	B	392	8.520	-8.773	22.767	1.00	19.94
20	ATOM	2624	C	VAL	B	392	9.615	-8.707	26.450	1.00	22.80
	ATOM	2625	O	VAL	B	392	10.336	-9.637	26.811	1.00	19.36
	ATOM	2626	N	TRP	B	393	9.617	-7.522	27.046	1.00	22.10
	ATOM	2627	CA	TRP	B	393	10.492	-7.241	28.171	1.00	23.20
	ATOM	2628	CB	TRP	B	393	10.388	-5.773	28.578	1.00	19.22
25	ATOM	2629	CG	TRP	B	393	11.056	-5.479	29.895	1.00	22.53
	ATOM	2630	CD2	TRP	B	393	12.453	-5.591	30.193	1.00	20.36
	ATOM	2631	CE2	TRP	B	393	12.624	-5.208	31.545	1.00	25.65
	ATOM	2632	CE3	TRP	B	393	13.578	-5.976	29.449	1.00	22.12
	ATOM	2633	CD1	TRP	B	393	10.452	-5.046	31.044	1.00	23.02
30	ATOM	2634	NE1	TRP	B	393	11.387	-4.881	32.037	1.00	24.91
	ATOM	2635	CZ2	TRP	B	393	13.876	-5.200	32.171	1.00	23.00
	ATOM	2636	CZ3	TRP	B	393	14.829	-5.968	30.072	1.00	23.98
	ATOM	2637	CH2	TRP	B	393	14.964	-5.582	31.423	1.00	23.20
	ATOM	2638	C	TRP	B	393	10.208	-8.114	29.388	1.00	24.36
35	ATOM	2639	O	TRP	B	393	11.128	-8.717	29.944	1.00	23.04
	ATOM	2640	N	ARG	B	394	8.952	-8.189	29.819	1.00	21.29
	ATOM	2641	CA	ARG	B	394	8.680	-9.003	30.990	1.00	22.43
	ATOM	2642	CB	ARG	B	394	7.365	-8.601	31.667	1.00	23.97
	ATOM	2643	CG	ARG	B	394	6.259	-8.149	30.759	1.00	26.16
40	ATOM	2644	CD	ARG	B	394	5.026	-7.727	31.574	1.00	20.86
	ATOM	2645	NE	ARG	B	394	3.817	-7.937	30.786	1.00	19.54
	ATOM	2646	CZ	ARG	B	394	3.327	-7.059	29.915	1.00	20.58
	ATOM	2647	NH1	ARG	B	394	3.944	-5.902	29.722	1.00	17.41
	ATOM	2648	NH2	ARG	B	394	2.229	-7.347	29.220	1.00	16.82
45	ATOM	2649	C	ARG	B	394	8.695	-10.502	30.713	1.00	21.78
	ATOM	2650	O	ARG	B	394	8.657	-11.294	31.648	1.00	23.44
	ATOM	2651	N	SER	B	395	8.767	-10.880	29.438	1.00	17.10
	ATOM	2652	CA	SER	B	395	8.805	-12.289	29.041	1.00	25.08
	ATOM	2653	CB	SER	B	395	8.206	-12.473	27.638	1.00	19.47
50	ATOM	2654	OG	SER	B	395	6.832	-12.136	27.619	1.00	21.73
	ATOM	2655	C	SER	B	395	10.239	-12.831	29.031	1.00	26.29
	ATOM	2656	O	SER	B	395	10.458	-14.030	28.854	1.00	23.75
	ATOM	2657	N	MET	B	396	11.206	-11.938	29.210	1.00	30.79
	ATOM	2658	CA	MET	B	396	12.620	-12.307	29.205	1.00	35.07
55	ATOM	2659	CB	MET	B	396	13.479	-11.063	29.423	1.00	33.84
	ATOM	2660	CG	MET	B	396	14.155	-10.569	28.171	1.00	36.88
	ATOM	2661	SD	MET	B	396	15.149	-9.127	28.491	1.00	40.96
	ATOM	2662	CE	MET	B	396	16.675	-9.849	28.998	1.00	39.67
	ATOM	2663	C	MET	B	396	12.983	-13.353	30.250	1.00	35.88
60	ATOM	2664	O	MET	B	396	13.828	-14.215	30.011	1.00	34.52
	ATOM	2665	N	GLU	B	397	12.348	-13.266	31.410	1.00	36.19

5	ATOM	2666	CA	GLU	B	397	12.604	-14.206	32.492	1.00	39.24
	ATOM	2667	CB	GLU	B	397	12.153	-13.605	33.821	1.00	44.38
	ATOM	2668	CG	GLU	B	397	12.983	-12.422	34.271	1.00	54.05
	ATOM	2669	CD	GLU	B	397	13.483	-12.587	35.686	1.00	56.78
10	ATOM	2670	OE1	GLU	B	397	13.380	-11.621	36.470	1.00	60.90
	ATOM	2671	OE2	GLU	B	397	13.975	-13.688	36.013	1.00	60.82
	ATOM	2672	C	GLU	B	397	11.878	-15.528	32.273	1.00	36.65
	ATOM	2673	O	GLU	B	397	12.021	-16.459	33.061	1.00	35.84
15	ATOM	2674	N	HIS	B	398	11.100	-15.609	31.202	1.00	32.14
	ATOM	2675	CA	HIS	B	398	10.347	-16.823	30.914	1.00	29.48
	ATOM	2676	CB	HIS	B	398	8.863	-16.567	31.178	1.00	29.87
	ATOM	2677	CG	HIS	B	398	8.582	-16.111	32.574	1.00	31.80
20	ATOM	2678	CD2	HIS	B	398	8.215	-16.801	33.678	1.00	29.12
	ATOM	2679	ND1	HIS	B	398	8.727	-14.799	32.972	1.00	33.27
	ATOM	2680	CE1	HIS	B	398	8.462	-14.701	34.262	1.00	32.19
	ATOM	2681	NE2	HIS	B	398	8.148	-15.902	34.714	1.00	33.48
25	ATOM	2682	C	HIS	B	398	10.556	-17.317	29.492	1.00	25.95
	ATOM	2683	O	HIS	B	398	9.637	-17.291	28.672	1.00	27.47
	ATOM	2684	N	PRO	B	399	11.771	-17.801	29.186	1.00	29.09
	ATOM	2685	CD	PRO	B	399	12.926	-17.922	30.096	1.00	29.93
30	ATOM	2686	CA	PRO	B	399	12.079	-18.300	27.845	1.00	27.40
	ATOM	2687	CB	PRO	B	399	13.434	-18.988	28.016	1.00	32.09
	ATOM	2688	CG	PRO	B	399	14.062	-18.284	29.170	1.00	30.81
	ATOM	2689	C	PRO	B	399	11.009	-19.246	27.319	1.00	29.76
35	ATOM	2690	O	PRO	B	399	10.552	-20.137	28.035	1.00	29.18
	ATOM	2691	N	GLY	B	400	10.601	-19.035	26.071	1.00	27.45
	ATOM	2692	CA	GLY	B	400	9.588	-19.884	25.466	1.00	26.93
	ATOM	2693	C	GLY	B	400	8.161	-19.537	25.849	1.00	26.73
40	ATOM	2694	O	GLY	B	400	7.220	-20.153	25.356	1.00	28.36
	ATOM	2695	N	LYS	B	401	7.996	-18.554	26.727	1.00	25.50
	ATOM	2696	CA	LYS	B	401	6.668	-18.139	27.165	1.00	23.45
	ATOM	2697	CB	LYS	B	401	6.435	-18.563	28.619	1.00	28.50
45	ATOM	2698	CG	LYS	B	401	6.476	-20.069	28.879	1.00	28.58
	ATOM	2699	CD	LYS	B	401	6.181	-20.353	30.349	1.00	35.47
	ATOM	2700	CE	LYS	B	401	6.073	-21.847	30.635	1.00	38.59
	ATOM	2701	NZ	LYS	B	401	6.073	-21.847	30.635	1.00	42.39
50	ATOM	2702	C	LYS	B	401	7.177	-22.611	29.989	1.00	21.78
	ATOM	2703	O	LYS	B	401	6.493	-16.622	27.060	1.00	21.45
	ATOM	2704	N	LEU	B	402	7.465	-15.872	27.035	1.00	21.45
	ATOM	2705	CA	LEU	B	402	5.241	-16.181	26.995	1.00	23.45
55	ATOM	2706	CB	LEU	B	402	4.929	-14.759	26.925	1.00	21.37
	ATOM	2707	CG	LEU	B	402	4.088	-14.449	25.689	1.00	18.47
	ATOM	2708	CD1	LEU	B	402	4.798	-14.673	24.360	1.00	16.89
	ATOM	2709	CD2	LEU	B	402	3.821	-14.395	23.211	1.00	21.23
60	ATOM	2710	C	LEU	B	402	6.011	-13.760	24.277	1.00	23.15
	ATOM	2711	O	LEU	B	402	4.147	-14.399	28.179	1.00	19.66
	ATOM	2712	N	LEU	B	403	3.024	-14.880	28.381	1.00	18.05
	ATOM	2713	CA	LEU	B	403	4.743	-13.559	29.019	1.00	19.54
65	ATOM	2714	CB	LEU	B	403	4.099	-13.148	30.259	1.00	20.21
	ATOM	2715	CG	LEU	B	403	5.155	-12.856	31.332	1.00	23.16
	ATOM	2716	CD1	LEU	B	403	4.639	-12.682	32.766	1.00	29.54
	ATOM	2717	CD2	LEU	B	403	5.519	-13.450	33.728	1.00	32.67
70	ATOM	2718	C	LEU	B	403	4.626	-11.213	33.138	1.00	32.38
	ATOM	2719	O	LEU	B	403	3.219	-11.918	30.043	1.00	20.42
	ATOM	2720	N	PHE	B	404	3.638	-10.787	30.291	1.00	19.18
	ATOM	2721	CA	PHE	B	404	2.003	-12.145	29.565	1.00	21.44
75	ATOM	2722	CB	PHE	B	404	1.066	-11.053	29.340	1.00	21.69
	ATOM	2723	CD	PHE	B	404	-0.199	-11.598	28.687	1.00	17.26

5	ATOM	2723	CG	PHE	B	404	-0.026	-11.897	27.227	1.00	19.75
	ATOM	2724	CD1	PHE	B	404	0.364	-13.167	26.801	1.00	17.90
	ATOM	2725	CD2	PHE	B	404	-0.210	-10.897	26.280	1.00	17.04
	ATOM	2726	CE1	PHE	B	404	0.572	-13.434	25.447	1.00	19.88
	ATOM	2727	CE2	PHE	B	404	-0.007	-11.148	24.924	1.00	18.47
10	ATOM	2728	CZ	PHE	B	404	0.386	-12.418	24.503	1.00	16.45
	ATOM	2729	C	PHE	B	404	0.768	-10.403	30.685	1.00	21.95
	ATOM	2730	O	PHE	B	404	0.656	-9.177	30.804	1.00	22.99
	ATOM	2731	N	ALA	B	405	0.670	-11.247	31.702	1.00	21.12
	ATOM	2732	CA	ALA	B	405	0.424	-10.814	33.066	1.00	22.43
15	ATOM	2733	CB	ALA	B	405	-1.074	-10.603	33.304	1.00	24.69
	ATOM	2734	C	ALA	B	405	0.959	-11.926	33.962	1.00	22.40
	ATOM	2735	O	ALA	B	405	1.133	-13.061	33.517	1.00	21.67
	ATOM	2736	N	PRO	B	406	1.246	-11.612	35.230	1.00	25.60
	ATOM	2737	CD	PRO	B	406	1.129	-10.294	35.878	1.00	23.65
20	ATOM	2738	CA	PRO	B	406	1.765	-12.632	36.148	1.00	25.91
	ATOM	2739	CB	PRO	B	406	1.899	-11.882	37.475	1.00	27.04
	ATOM	2740	CG	PRO	B	406	2.017	-10.431	37.068	1.00	26.56
	ATOM	2741	C	PRO	B	406	0.876	-13.873	36.259	1.00	25.12
	ATOM	2742	O	PRO	B	406	1.368	-14.967	36.538	1.00	28.92
25	ATOM	2743	N	ASN	B	407	-0.426	-13.713	36.039	1.00	23.53
	ATOM	2744	CA	ASN	B	407	-1.345	-14.852	36.109	1.00	24.09
	ATOM	2745	CB	ASN	B	407	-2.553	-14.526	36.986	1.00	24.08
	ATOM	2746	CG	ASN	B	407	-3.327	-13.328	36.486	1.00	26.72
	ATOM	2747	OD1	ASN	B	407	-2.851	-12.574	35.635	1.00	22.65
30	ATOM	2748	ND2	ASN	B	407	-4.528	-13.140	37.019	1.00	26.46
	ATOM	2749	C	ASN	B	407	-1.820	-15.231	34.714	1.00	26.91
	ATOM	2750	O	ASN	B	407	-2.859	-15.870	34.548	1.00	28.68
	ATOM	2751	N	LEU	B	408	-1.059	-14.816	33.708	1.00	27.28
	ATOM	2752	CA	LEU	B	408	-1.387	-15.124	32.327	1.00	27.23
35	ATOM	2753	CB	LEU	B	408	-2.247	-14.030	31.699	1.00	26.61
	ATOM	2754	CG	LEU	B	408	-2.815	-14.464	30.341	1.00	27.51
	ATOM	2755	CD1	LEU	B	408	-3.702	-15.692	30.546	1.00	28.75
	ATOM	2756	CD2	LEU	B	408	-3.598	-13.330	29.694	1.00	25.48
	ATOM	2757	C	LEU	B	408	-0.113	-15.316	31.514	1.00	27.56
40	ATOM	2758	O	LEU	B	408	0.247	-14.465	30.695	1.00	26.86
	ATOM	2759	N	LEU	B	409	0.553	-16.426	31.759	1.00	27.54
	ATOM	2760	CA	LEU	B	409	1.786	-16.774	31.065	1.00	31.96
	ATOM	2761	CB	LEU	B	409	2.786	-17.355	32.058	1.00	31.88
	ATOM	2762	CG	LEU	B	409	4.186	-17.703	31.562	1.00	37.72
45	ATOM	2763	CD1	LEU	B	409	4.773	-16.551	30.770	1.00	39.57
	ATOM	2764	CD2	LEU	B	409	5.066	-18.018	32.758	1.00	41.72
	ATOM	2765	C	LEU	B	409	1.401	-17.805	30.009	1.00	31.53
	ATOM	2766	O	LEU	B	409	0.921	-18.892	30.340	1.00	32.67
	ATOM	2767	N	LEU	B	410	1.604	-17.465	28.746	1.00	29.58
50	ATOM	2768	CA	LEU	B	410	1.228	-18.361	27.660	1.00	31.55
	ATOM	2769	CB	LEU	B	410	0.192	-17.672	26.762	1.00	29.83
	ATOM	2770	CG	LEU	B	410	-1.047	-17.080	27.452	1.00	28.55
	ATOM	2771	CD1	LEU	B	410	-1.770	-16.135	26.501	1.00	26.92
	ATOM	2772	CD2	LEU	B	410	-1.979	-18.200	27.891	1.00	30.49
55	ATOM	2773	C	LEU	B	410	2.397	-18.839	26.814	1.00	33.88
	ATOM	2774	O	LEU	B	410	3.427	-18.170	26.726	1.00	36.49
	ATOM	2775	N	ASP	B	411	2.238	-20.013	26.206	1.00	38.80
	ATOM	2776	CA	ASP	B	411	3.275	-20.562	25.336	1.00	38.39
	ATOM	2777	CB	ASP	B	411	3.657	-21.990	25.752	1.00	44.53
60	ATOM	2778	CG	ASP	B	411	2.476	-22.943	25.749	1.00	44.90
	ATOM	2779	OD1	ASP	B	411	1.773	-23.035	24.719	1.00	45.70

							2.254	-23.603	26.786	1.00	50.54
5	ATOM	2780	OD2	ASP	B	411	2.745	-20.551	23.909	1.00	38.57
	ATOM	2781	C	ASP	B	411	1.549	-20.341	23.686	1.00	36.48
	ATOM	2782	O	ASP	B	411	3.635	-20.777	22.949	1.00	36.85
	ATOM	2783	N	ARG	B	412	3.259	-20.763	21.541	1.00	38.32
	ATOM	2784	CA	ARG	B	412	4.488	-21.083	20.675	1.00	38.69
10	ATOM	2785	CB	ARG	B	412	4.361	-22.314	19.799	1.00	40.05
	ATOM	2786	CG	ARG	B	412	5.644	-22.552	19.012	1.00	42.98
	ATOM	2787	CD	ARG	B	412	5.540	-22.099	17.626	1.00	40.95
	ATOM	2788	NE	ARG	B	412	4.649	-22.559	16.753	1.00	41.11
	ATOM	2789	CZ	ARG	B	412	3.777	-23.490	17.115	1.00	44.01
15	ATOM	2790	NH1	ARG	B	412	4.632	-22.091	15.515	1.00	41.28
	ATOM	2791	NH2	ARG	B	412	2.107	-21.712	21.217	1.00	37.64
	ATOM	2792	C	ARG	B	412	1.287	-21.427	20.343	1.00	36.51
	ATOM	2793	O	ARG	B	412	2.041	-22.834	21.923	1.00	35.32
	ATOM	2794	N	ASN	B	413	0.974	-23.798	21.688	1.00	36.68
20	ATOM	2795	CA	ASN	B	413	1.170	-25.035	22.570	1.00	37.54
	ATOM	2796	CB	ASN	B	413	2.017	-26.100	21.901	1.00	43.56
	ATOM	2797	CG	ASN	B	413	2.309	-26.022	20.704	1.00	46.11
	ATOM	2798	OD1	ASN	B	413	2.418	-27.104	22.671	1.00	47.04
	ATOM	2799	ND2	ASN	B	413	-0.383	-23.168	21.982	1.00	34.01
25	ATOM	2800	C	ASN	B	413	-1.349	-23.372	21.247	1.00	32.43
	ATOM	2801	O	ASN	B	413	-0.447	-22.397	23.063	1.00	32.85
	ATOM	2802	N	GLN	B	414	-1.685	-21.741	23.449	1.00	31.91
	ATOM	2803	CA	GLN	B	414	-1.558	-21.172	24.863	1.00	33.17
	ATOM	2804	CB	GLN	B	414	-1.528	-22.242	25.948	1.00	32.31
30	ATOM	2805	CG	GLN	B	414	-1.293	-21.667	27.327	1.00	34.63
	ATOM	2806	CD	GLN	B	414	-0.176	-21.277	27.666	1.00	33.23
	ATOM	2807	OE1	GLN	B	414	-2.349	-21.606	28.131	1.00	34.56
	ATOM	2808	NE2	GLN	B	414	-2.052	-20.638	22.463	1.00	29.57
	ATOM	2809	C	GLN	B	414	-3.195	-20.204	22.409	1.00	31.32
35	ATOM	2810	O	GLN	B	414	-1.077	-20.190	21.682	1.00	30.96
	ATOM	2811	N	GLY	B	415	-1.350	-19.160	20.697	1.00	34.27
	ATOM	2812	CA	GLY	B	415	-2.184	-19.725	19.562	1.00	35.27
	ATOM	2813	C	GLY	B	415	-2.918	-19.000	18.887	1.00	33.20
	ATOM	2814	O	GLY	B	415	-2.070	-21.031	19.354	1.00	35.28
40	ATOM	2815	N	LYS	B	416	-2.819	-21.707	18.299	1.00	38.26
	ATOM	2816	CA	LYS	B	416	-2.398	-23.177	18.201	1.00	38.00
	ATOM	2817	CB	LYS	B	416	-0.973	-23.407	17.736	1.00	40.05
	ATOM	2818	CG	LYS	B	416	-0.405	-24.668	18.369	1.00	44.10
	ATOM	2819	CD	LYS	B	416	0.306	-25.541	17.346	1.00	41.85
45	ATOM	2820	CE	LYS	B	416	1.286	-24.760	16.542	1.00	45.63
	ATOM	2821	NZ	LYS	B	416	-4.321	-21.645	18.559	1.00	36.93
	ATOM	2822	C	LYS	B	416	-5.121	-21.790	17.638	1.00	38.36
	ATOM	2823	O	LYS	B	416	-4.698	-21.430	19.817	1.00	37.10
	ATOM	2824	N	CYS	B	417	-6.106	-21.371	20.196	1.00	36.46
50	ATOM	2825	CA	CYS	B	417	-6.218	-21.226	21.717	1.00	39.01
	ATOM	2826	CB	CYS	B	417	-5.674	-22.710	22.612	1.00	43.81
	ATOM	2827	SG	CYS	B	417	-6.899	-20.277	19.491	1.00	35.19
	ATOM	2828	C	CYS	B	417	-8.127	-20.296	19.485	1.00	33.92
	ATOM	2829	O	CYS	B	417	-6.195	-19.316	18.906	1.00	36.04
55	ATOM	2830	N	VAL	B	418	-6.838	-18.236	18.163	1.00	34.59
	ATOM	2831	CA	VAL	B	418	-6.525	-16.850	18.775	1.00	34.87
	ATOM	2832	CB	VAL	B	418	-6.831	-15.763	17.765	1.00	35.32
	ATOM	2833	CG1	VAL	B	418	-7.350	-16.630	20.036	1.00	33.65
	ATOM	2834	CG2	VAL	B	418	-6.241	-18.317	16.764	1.00	34.17
60	ATOM	2835	C	VAL	B	418	-5.020	-18.323	16.611	1.00	32.73
	ATOM	2836	O	VAL	B	418					

5	ATOM	2837	N	GLU	B	419	-7.084	-18.388	15.740	1.00	33.44
	ATOM	2838	CA	GLU	B	419	-6.554	-18.500	14.390	1.00	34.52
	ATOM	2839	CB	GLU	B	419	-7.681	-18.722	13.380	1.00	36.21
	ATOM	2840	CG	GLU	B	419	-8.597	-17.538	13.166	1.00	44.19
	ATOM	2841	CD	GLU	B	419	-9.477	-17.723	11.946	1.00	48.47
10	ATOM	2842	OE1	GLU	B	419	-9.157	-18.605	11.119	1.00	51.04
	ATOM	2843	OE2	GLU	B	419	-10.484	-16.993	11.813	1.00	48.91
	ATOM	2844	C	GLU	B	419	-5.717	-17.289	13.997	1.00	32.89
	ATOM	2845	O	GLU	B	419	-6.156	-16.144	14.123	1.00	31.09
	ATOM	2846	N	GLY	B	420	-4.501	-17.562	13.535	1.00	32.84
15	ATOM	2847	CA	GLY	B	420	-3.594	-16.506	13.122	1.00	34.37
	ATOM	2848	C	GLY	B	420	-2.722	-15.955	14.240	1.00	35.30
	ATOM	2849	O	GLY	B	420	-1.745	-15.246	13.975	1.00	35.94
	ATOM	2850	N	MET	B	421	-3.052	-16.285	15.486	1.00	30.08
	ATOM	2851	CA	MET	B	421	-2.289	-15.780	16.625	1.00	29.22
20	ATOM	2852	CB	MET	B	421	-3.108	-15.922	17.914	1.00	22.54
	ATOM	2853	CG	MET	B	421	-2.469	-15.270	19.124	1.00	23.82
	ATOM	2854	SD	MET	B	421	-2.124	-13.494	18.872	1.00	28.40
	ATOM	2855	CE	MET	B	421	-3.697	-12.800	19.233	1.00	24.67
	ATOM	2856	C	MET	B	421	-0.912	-16.416	16.821	1.00	29.67
25	ATOM	2857	O	MET	B	421	0.022	-15.751	17.269	1.00	29.76
	ATOM	2858	N	VAL	B	422	-0.766	-17.694	16.484	1.00	30.63
	ATOM	2859	CA	VAL	B	422	0.524	-18.338	16.675	1.00	29.90
	ATOM	2860	CB	VAL	B	422	0.482	-19.835	16.273	1.00	35.74
	ATOM	2861	CG1	VAL	B	422	0.514	-19.992	14.753	1.00	37.64
30	ATOM	2862	CG2	VAL	B	422	1.659	-20.555	16.897	1.00	31.68
	ATOM	2863	C	VAL	B	422	1.669	-17.640	15.935	1.00	28.64
	ATOM	2864	O	VAL	B	422	2.788	-17.571	16.441	1.00	26.15
	ATOM	2865	N	GLU	B	423	1.402	-17.113	14.747	1.00	28.70
	ATOM	2866	CA	GLU	B	423	2.454	-16.435	13.997	1.00	31.34
35	ATOM	2867	CB	GLU	B	423	1.963	-16.050	12.596	1.00	36.21
	ATOM	2868	CG	GLU	B	423	0.502	-16.376	12.325	1.00	45.83
	ATOM	2869	CD	GLU	B	423	0.250	-17.865	12.144	1.00	46.71
	ATOM	2870	OE1	GLU	B	423	-0.746	-18.368	12.706	1.00	45.97
	ATOM	2871	OE2	GLU	B	423	1.045	-18.530	11.442	1.00	50.05
40	ATOM	2872	C	GLU	B	423	2.928	-15.186	14.744	1.00	30.57
	ATOM	2873	O	GLU	B	423	4.119	-14.870	14.759	1.00	26.59
	ATOM	2874	N	ILE	B	424	2.001	-14.478	15.378	1.00	26.19
	ATOM	2875	CA	ILE	B	424	2.381	-13.279	16.111	1.00	26.23
	ATOM	2876	CB	ILE	B	424	1.134	-12.435	16.452	1.00	29.33
45	ATOM	2877	CG2	ILE	B	424	1.492	-11.315	17.425	1.00	30.91
	ATOM	2878	CG1	ILE	B	424	0.584	-11.817	15.160	1.00	29.09
	ATOM	2879	CD1	ILE	B	424	-0.895	-11.514	15.187	1.00	30.51
	ATOM	2880	C	ILE	B	424	3.153	-13.673	17.370	1.00	24.22
	ATOM	2881	O	ILE	B	424	4.152	-13.037	17.725	1.00	21.05
50	ATOM	2882	N	PHE	B	425	2.708	-14.746	18.023	1.00	21.71
	ATOM	2883	CA	PHE	B	425	3.370	-15.236	19.223	1.00	18.85
	ATOM	2884	CB	PHE	B	425	2.650	-16.479	19.768	1.00	22.98
	ATOM	2885	CG	PHE	B	425	1.580	-16.183	20.795	1.00	22.17
	ATOM	2886	CD1	PHE	B	425	1.287	-17.112	21.792	1.00	25.47
55	ATOM	2887	CD2	PHE	B	425	0.843	-15.001	20.747	1.00	26.30
	ATOM	2888	CE1	PHE	B	425	0.273	-16.871	22.724	1.00	24.33
	ATOM	2889	CE2	PHE	B	425	-0.174	-14.749	21.676	1.00	25.03
	ATOM	2890	CZ	PHE	B	425	-0.459	-15.684	22.663	1.00	26.44
	ATOM	2891	C	PHE	B	425	4.817	-15.610	18.885	1.00	20.00
60	ATOM	2892	O	PHE	B	425	5.741	-15.292	19.636	1.00	21.15
	ATOM	2893	N	ASP	B	426	5.023	-16.281	17.754	1.00	19.87

5	ATOM	2894	CA	ASP	B	426	6.378	-16.685	17.377	1.00	23.20
	ATOM	2895	CB	ASP	B	426	6.364	-17.510	16.090	1.00	26.53
	ATOM	2896	CG	ASP	B	426	5.992	-18.965	16.335	1.00	34.28
	ATOM	2897	OD1	ASP	B	426	6.242	-19.467	17.455	1.00	35.24
	ATOM	2898	OD2	ASP	B	426	5.448	-19.600	15.409	1.00	31.49
10	ATOM	2899	C	ASP	B	426	7.302	-15.489	17.198	1.00	21.84
	ATOM	2900	O	ASP	B	426	8.465	-15.526	17.593	1.00	21.55
	ATOM	2901	N	MET	B	427	6.788	-14.429	16.591	1.00	20.12
	ATOM	2902	CA	MET	B	427	7.597	-13.234	16.382	1.00	21.02
	ATOM	2903	CB	MET	B	427	6.836	-12.228	15.520	1.00	18.53
15	ATOM	2904	CG	MET	B	427	6.864	-12.559	14.038	1.00	27.92
	ATOM	2905	SD	MET	B	427	6.011	-11.341	13.024	1.00	32.84
	ATOM	2906	CE	MET	B	427	4.363	-11.532	13.581	1.00	33.63
	ATOM	2907	C	MET	B	427	7.945	-12.616	17.732	1.00	17.42
	ATOM	2908	O	MET	B	427	9.073	-12.180	17.950	1.00	22.09
20	ATOM	2909	N	LEU	B	428	6.968	-12.597	18.634	1.00	20.47
	ATOM	2910	CA	LEU	B	428	7.157	-12.033	19.968	1.00	20.13
	ATOM	2911	CB	LEU	B	428	5.812	-11.964	20.706	1.00	17.58
	ATOM	2912	CG	LEU	B	428	4.852	-10.887	20.179	1.00	18.41
	ATOM	2913	CD1	LEU	B	428	3.443	-11.155	20.687	1.00	11.95
25	ATOM	2914	CD2	LEU	B	428	5.324	-9.505	20.631	1.00	17.80
	ATOM	2915	C	LEU	B	428	8.159	-12.856	20.767	1.00	20.68
	ATOM	2916	O	LEU	B	428	9.028	-12.305	21.445	1.00	20.45
	ATOM	2917	N	LEU	B	429	8.037	-14.178	20.679	1.00	20.35
	ATOM	2918	CA	LEU	B	429	8.938	-15.082	21.382	1.00	19.82
30	ATOM	2919	CB	LEU	B	429	8.470	-16.532	21.211	1.00	23.13
	ATOM	2920	CG	LEU	B	429	7.189	-16.839	21.997	1.00	21.85
	ATOM	2921	CD1	LEU	B	429	6.551	-18.123	21.494	1.00	25.39
	ATOM	2922	CD2	LEU	B	429	7.537	-16.944	23.475	1.00	24.91
	ATOM	2923	C	LEU	B	429	10.361	-14.936	20.865	1.00	20.74
35	ATOM	2924	O	LEU	B	429	11.318	-14.968	21.638	1.00	21.02
	ATOM	2925	N	ALA	B	430	10.495	-14.770	19.554	1.00	21.40
	ATOM	2926	CA	ALA	B	430	11.808	-14.609	18.947	1.00	22.77
	ATOM	2927	CB	ALA	B	430	11.677	-14.596	17.432	1.00	21.11
	ATOM	2928	C	ALA	B	430	12.467	-13.315	19.440	1.00	22.40
40	ATOM	2929	O	ALA	B	430	13.670	-13.277	19.713	1.00	20.62
	ATOM	2930	N	THR	B	431	11.670	-12.258	19.567	1.00	21.09
	ATOM	2931	CA	THR	B	431	12.183	-10.974	20.021	1.00	22.67
	ATOM	2932	CB	THR	B	431	11.128	-9.866	19.863	1.00	23.77
	ATOM	2933	OG1	THR	B	431	10.572	-9.936	18.547	1.00	23.84
45	ATOM	2934	CG2	THR	B	431	11.762	-8.489	20.073	1.00	21.78
	ATOM	2935	C	THR	B	431	12.603	-11.037	21.480	1.00	21.98
	ATOM	2936	O	THR	B	431	13.595	-10.429	21.879	1.00	19.85
	ATOM	2937	N	SER	B	432	11.844	-11.773	22.280	1.00	24.24
	ATOM	2938	CA	SER	B	432	12.169	-11.906	23.693	1.00	26.96
50	ATOM	2939	CB	SER	B	432	11.055	-12.661	24.423	1.00	28.00
	ATOM	2940	OG	SER	B	432	11.404	-12.888	25.776	1.00	30.31
	ATOM	2941	C	SER	B	432	13.491	-12.660	23.820	1.00	27.67
	ATOM	2942	O	SER	B	432	14.305	-12.377	24.701	1.00	23.78
	ATOM	2943	N	SER	B	433	13.691	-13.628	22.932	1.00	29.27
55	ATOM	2944	CA	SER	B	433	14.914	-14.421	22.928	1.00	31.96
	ATOM	2945	CB	SER	B	433	14.790	-15.575	21.938	1.00	30.84
	ATOM	2946	OG	SER	B	433	14.761	-16.808	22.625	1.00	38.26
	ATOM	2947	C	SER	B	433	16.104	-13.550	22.548	1.00	31.47
	ATOM	2948	O	SER	B	433	17.204	-13.701	23.087	1.00	28.43
60	ATOM	2949	N	ARG	B	434	15.878	-12.641	21.607	1.00	29.55
	ATOM	2950	CA	ARG	B	434	16.926	-11.739	21.165	1.00	29.40

5	ATOM	2951	CB	ARG	B	434	16.437	-10.912	19.977	1.00	31.56
	ATOM	2952	CG	ARG	B	434	17.428	-9.868	19.493	1.00	36.76
	ATOM	2953	CD	ARG	B	434	18.694	-10.502	18.919	1.00	37.76
	ATOM	2954	NE	ARG	B	434	19.654	-9.479	18.516	1.00	39.50
	ATOM	2955	CZ	ARG	B	434	20.965	-9.673	18.418	1.00	44.17
10	ATOM	2956	NH1	ARG	B	434	21.492	-10.861	18.696	1.00	43.17
	ATOM	2957	NH2	ARG	B	434	21.750	-8.671	18.048	1.00	43.05
	ATOM	2958	C	ARG	B	434	17.328	-10.827	22.326	1.00	29.15
	ATOM	2959	O	ARG	B	434	18.515	-10.612	22.569	1.00	28.82
	ATOM	2960	N	PHE	B	435	16.337	-10.297	23.039	1.00	24.88
15	ATOM	2961	CA	PHE	B	435	16.600	-9.422	24.186	1.00	25.74
	ATOM	2962	CB	PHE	B	435	15.278	-8.972	24.825	1.00	26.53
	ATOM	2963	CG	PHE	B	435	14.656	-7.758	24.183	1.00	30.94
	ATOM	2964	CD1	PHE	B	435	15.118	-7.271	22.966	1.00	32.65
	ATOM	2965	CD2	PHE	B	435	13.592	-7.108	24.797	1.00	33.60
20	ATOM	2966	CE1	PHE	B	435	14.529	-6.155	22.372	1.00	36.84
	ATOM	2967	CE2	PHE	B	435	12.997	-5.989	24.208	1.00	34.96
	ATOM	2968	CZ	PHE	B	435	13.468	-5.516	22.995	1.00	31.64
	ATOM	2969	C	PHE	B	435	17.426	-10.184	25.233	1.00	25.39
	ATOM	2970	O	PHE	B	435	18.414	-9.675	25.764	1.00	22.59
25	ATOM	2971	N	ARG	B	436	16.999	-11.405	25.528	1.00	24.58
	ATOM	2972	CA	ARG	B	436	17.675	-12.253	26.503	1.00	30.25
	ATOM	2973	CB	ARG	B	436	16.898	-13.569	26.662	1.00	33.32
	ATOM	2974	CG	ARG	B	436	17.232	-14.358	27.915	1.00	38.17
	ATOM	2975	CD	ARG	B	436	16.135	-15.367	28.260	1.00	37.27
30	ATOM	2976	NE	ARG	B	436	15.646	-16.085	27.086	1.00	43.92
	ATOM	2977	CZ	ARG	B	436	14.433	-15.923	26.557	1.00	46.68
	ATOM	2978	NH1	ARG	B	436	13.578	-15.061	27.097	1.00	45.59
	ATOM	2979	NH2	ARG	B	436	14.074	-16.620	25.486	1.00	46.25
	ATOM	2980	C	ARG	B	436	19.110	-12.531	26.048	1.00	29.82
35	ATOM	2981	O	ARG	B	436	20.057	-12.397	26.823	1.00	28.76
	ATOM	2982	N	AMET	B	437	19.269	-12.921	24.789	0.50	30.27
	ATOM	2983	N	BMET	B	437	19.252	-12.906	24.781	0.50	31.41
	ATOM	2984	CA	AMET	B	437	20.591	-13.212	24.253	0.50	31.98
	ATOM	2985	CA	BMET	B	437	20.547	-13.206	24.183	0.50	33.77
40	ATOM	2986	CB	AMET	B	437	20.489	-13.646	22.788	0.50	31.34
	ATOM	2987	CB	BMET	B	437	20.348	-13.595	22.714	0.50	35.88
	ATOM	2988	CG	AMET	B	437	20.179	-15.127	22.592	0.50	33.62
	ATOM	2989	CG	BMET	B	437	21.605	-13.594	21.861	0.50	40.47
	ATOM	2990	SD	AMET	B	437	20.354	-16.099	24.109	0.50	35.21
45	ATOM	2991	SD	BMET	B	437	21.247	-13.937	20.115	0.50	46.79
	ATOM	2992	CE	AMET	B	437	22.155	-16.194	24.259	0.50	33.20
	ATOM	2993	CE	BMET	B	437	21.837	-15.632	19.976	0.50	43.22
	ATOM	2994	C	AMET	B	437	21.498	-11.993	24.366	0.50	33.33
	ATOM	2995	C	BMET	B	437	21.487	-12.005	24.289	0.50	34.45
50	ATOM	2996	O	AMET	B	437	22.702	-12.123	24.594	0.50	33.54
	ATOM	2997	O	BMET	B	437	22.699	-12.162	24.438	0.50	34.43
	ATOM	2998	N	MET	B	438	20.913	-10.809	24.215	1.00	32.07
	ATOM	2999	CA	MET	B	438	21.674	-9.560	24.298	1.00	32.48
	ATOM	3000	CB	MET	B	438	20.930	-8.437	23.578	1.00	29.74
55	ATOM	3001	CG	MET	B	438	21.161	-8.364	22.093	1.00	36.73
	ATOM	3002	SD	MET	B	438	20.425	-6.849	21.462	1.00	38.21
	ATOM	3003	CE	MET	B	438	21.693	-5.657	21.943	1.00	35.91
	ATOM	3004	C	MET	B	438	21.877	-9.122	25.738	1.00	28.81
	ATOM	3005	O	MET	B	438	22.686	-8.240	26.013	1.00	30.13
60	ATOM	3006	N	ASN	B	439	21.120	-9.721	26.646	1.00	27.14
	ATOM	3007	CA	ASN	B	439	21.199	-9.359	28.038	1.00	27.34

5	ATOM	3008	CB	ASN	B	439	22.592	-9.524	28.598	1.00	34.85
	ATOM	3009	CG	ASN	B	439	22.624	-9.480	30.080	1.00	38.58
	ATOM	3010	OD1	ASN	B	439	21.584	-9.620	30.724	1.00	42.99
	ATOM	3011	ND2	ASN	B	439	23.801	-9.260	30.666	1.00	41.14
	ATOM	3012	C	ASN	B	439	20.745	-7.903	28.212	1.00	26.24
10	ATOM	3013	O	ASN	B	439	21.396	-7.106	28.891	1.00	19.76
	ATOM	3014	N	LEU	B	440	19.625	-7.564	27.573	1.00	24.90
	ATOM	3015	CA	LEU	B	440	19.061	-6.214	27.633	1.00	25.04
	ATOM	3016	CB	LEU	B	440	17.761	-6.157	26.818	1.00	22.36
	ATOM	3017	CG	LEU	B	440	17.087	-4.786	26.740	1.00	26.33
15	ATOM	3018	CD1	LEU	B	440	17.958	-3.843	25.923	1.00	28.33
	ATOM	3019	CD2	LEU	B	440	15.704	-4.914	26.111	1.00	24.81
	ATOM	3020	C	LEU	B	440	18.782	-5.785	29.074	1.00	24.71
	ATOM	3021	O	LEU	B	440	18.131	-6.504	29.830	1.00	26.96
	ATOM	3022	N	GLN	B	441	19.268	-4.609	29.452	1.00	25.54
20	ATOM	3023	CA	GLN	B	441	19.060	-4.099	30.807	1.00	25.82
	ATOM	3024	CB	GLN	B	441	20.250	-3.231	31.234	1.00	30.41
	ATOM	3025	CG	GLN	B	441	21.572	-3.956	31.228	1.00	30.50
	ATOM	3026	CD	GLN	B	441	21.610	-5.028	32.279	1.00	32.75
	ATOM	3027	OE1	GLN	B	441	21.539	-4.772	33.473	1.00	36.52
25	ATOM	3028	NE2	GLN	B	441	21.703	-6.288	31.823	1.00	31.09
	ATOM	3029	C	GLN	B	441	17.789	-3.265	30.883	1.00	26.93
	ATOM	3030	O	GLN	B	441	17.303	-2.768	29.866	1.00	25.40
	ATOM	3031	N	GLY	B	442	17.266	-3.105	32.096	1.00	24.56
	ATOM	3032	CA	GLY	B	442	16.058	-2.327	32.293	1.00	22.82
30	ATOM	3033	C	GLY	B	442	16.217	-0.873	31.885	1.00	24.19
	ATOM	3034	O	GLY	B	442	15.290	-0.279	31.341	1.00	20.21
	ATOM	3035	N	GLU	B	443	17.387	-0.293	32.141	1.00	22.92
	ATOM	3036	CA	GLU	B	443	17.635	1.102	31.778	1.00	23.33
	ATOM	3037	CB	GLU	B	443	18.960	1.590	32.378	1.00	24.26
35	ATOM	3038	CG	GLU	B	443	19.005	1.525	33.895	1.00	32.31
	ATOM	3039	CD	GLU	B	443	19.701	0.270	34.402	1.00	37.68
	ATOM	3040	OE1	GLU	B	443	19.343	-0.841	33.948	1.00	35.23
	ATOM	3041	OE2	GLU	B	443	20.607	0.394	35.252	1.00	42.47
	ATOM	3042	C	GLU	B	443	17.662	1.278	30.262	1.00	23.08
40	ATOM	3043	O	GLU	B	443	17.265	2.328	29.747	1.00	21.80
	ATOM	3044	N	GLU	B	444	18.128	0.253	29.552	1.00	21.16
	ATOM	3045	CA	GLU	B	444	18.182	0.302	28.093	1.00	22.60
	ATOM	3046	CB	GLU	B	444	19.046	-0.834	27.545	1.00	20.89
	ATOM	3047	CG	GLU	B	444	20.545	-0.617	27.705	1.00	23.24
45	ATOM	3048	CD	GLU	B	444	21.340	-1.869	27.393	1.00	22.11
	ATOM	3049	OE1	GLU	B	444	20.817	-2.978	27.629	1.00	20.89
	ATOM	3050	OE2	GLU	B	444	22.488	-1.746	26.914	1.00	25.49
	ATOM	3051	C	GLU	B	444	16.758	0.155	27.552	1.00	21.06
	ATOM	3052	O	GLU	B	444	16.377	0.822	26.597	1.00	23.73
50	ATOM	3053	N	PHE	B	445	15.987	-0.730	28.176	1.00	19.01
	ATOM	3054	CA	PHE	B	445	14.600	-0.969	27.792	1.00	19.44
	ATOM	3055	CB	PHE	B	445	13.989	-2.067	28.675	1.00	18.12
	ATOM	3056	CG	PHE	B	445	12.483	-2.055	28.709	1.00	18.13
	ATOM	3057	CD1	PHE	B	445	11.746	-2.386	27.575	1.00	18.34
55	ATOM	3058	CD2	PHE	B	445	11.802	-1.694	29.872	1.00	16.59
	ATOM	3059	CE1	PHE	B	445	10.346	-2.359	27.592	1.00	17.15
	ATOM	3060	CE2	PHE	B	445	10.406	-1.662	29.903	1.00	21.99
	ATOM	3061	CZ	PHE	B	445	9.674	-1.997	28.755	1.00	16.01
	ATOM	3062	C	PHE	B	445	13.758	0.304	27.888	1.00	15.87
60	ATOM	3063	O	PHE	B	445	13.008	0.617	26.966	1.00	20.27
	ATOM	3064	N	VAL	B	446	13.872	1.044	28.986	1.00	15.90



5	ATOM	3065	CA	VAL	B	446	13.074	2.269	29.112	1.00	16.78
	ATOM	3066	CB	VAL	B	446	13.165	2.895	30.531	1.00	18.32
	ATOM	3067	CG1	VAL	B	446	12.574	1.923	31.551	1.00	21.14
	ATOM	3068	CG2	VAL	B	446	14.598	3.251	30.879	1.00	21.04
	ATOM	3069	C	VAL	B	446	13.450	3.295	28.051	1.00	17.91
10	ATOM	3070	O	VAL	B	446	12.596	4.028	27.561	1.00	19.37
	ATOM	3071	N	CYS	B	447	14.723	3.335	27.674	1.00	18.81
	ATOM	3072	CA	CYS	B	447	15.161	4.255	26.635	1.00	17.34
	ATOM	3073	CB	CYS	B	447	16.682	4.224	26.512	1.00	19.33
	ATOM	3074	SG	CYS	B	447	17.538	5.134	27.798	1.00	23.60
15	ATOM	3075	C	CYS	B	447	14.537	3.826	25.301	1.00	18.09
	ATOM	3076	O	CYS	B	447	13.988	4.643	24.563	1.00	17.52
	ATOM	3077	N	LEU	B	448	14.623	2.533	25.006	1.00	15.60
	ATOM	3078	CA	LEU	B	448	14.072	1.994	23.767	1.00	16.67
	ATOM	3079	CB	LEU	B	448	14.328	0.490	23.684	1.00	14.82
20	ATOM	3080	CG	LEU	B	448	15.730	0.009	23.301	1.00	23.57
	ATOM	3081	CD1	LEU	B	448	15.722	-1.522	23.169	1.00	21.61
	ATOM	3082	CD2	LEU	B	448	16.167	0.658	21.986	1.00	18.92
	ATOM	3083	C	LEU	B	448	12.573	2.249	23.652	1.00	15.98
	ATOM	3084	O	LEU	B	448	12.078	2.633	22.590	1.00	18.91
25	ATOM	3085	N	LYS	B	449	11.849	2.037	24.745	1.00	17.94
	ATOM	3086	CA	LYS	B	449	10.405	2.232	24.733	1.00	16.66
	ATOM	3087	CB	LYS	B	449	9.796	1.745	26.047	1.00	16.45
	ATOM	3088	CG	LYS	B	449	8.285	1.861	26.115	1.00	16.12
	ATOM	3089	CD	LYS	B	449	7.730	0.952	27.193	1.00	19.09
30	ATOM	3090	CE	LYS	B	449	8.201	1.380	28.580	1.00	17.04
	ATOM	3091	NZ	LYS	B	449	7.159	1.088	29.593	1.00	17.25
	ATOM	3092	C	LYS	B	449	10.058	3.696	24.486	1.00	18.78
	ATOM	3093	O	LYS	B	449	9.103	3.996	23.769	1.00	14.84
	ATOM	3094	N	SER	B	450	10.837	4.610	25.059	1.00	14.50
35	ATOM	3095	CA	SER	B	450	10.591	6.032	24.849	1.00	17.11
	ATOM	3096	CB	SER	B	450	11.440	6.866	25.815	1.00	21.20
	ATOM	3097	OG	SER	B	450	10.859	6.868	27.108	1.00	30.66
	ATOM	3098	C	SER	B	450	10.921	6.418	23.405	1.00	17.84
	ATOM	3099	O	SER	B	450	10.279	7.292	22.821	1.00	18.82
40	ATOM	3100	N	ILE	B	451	11.926	5.768	22.828	1.00	16.88
	ATOM	3101	CA	ILE	B	451	12.305	6.063	21.450	1.00	17.11
	ATOM	3102	CB	ILE	B	451	13.564	5.268	21.025	1.00	16.69
	ATOM	3103	CG2	ILE	B	451	13.724	5.298	19.505	1.00	19.31
	ATOM	3104	CG1	ILE	B	451	14.804	5.897	21.676	1.00	18.96
45	ATOM	3105	CD1	ILE	B	451	16.083	5.130	21.431	1.00	18.98
	ATOM	3106	C	ILE	B	451	11.142	5.711	20.527	1.00	18.09
	ATOM	3107	O	ILE	B	451	10.820	6.464	19.608	1.00	17.07
	ATOM	3108	N	ILE	B	452	10.505	4.571	20.786	1.00	18.13
	ATOM	3109	CA	ILE	B	452	9.373	4.137	19.976	1.00	16.77
50	ATOM	3110	CB	ILE	B	452	8.804	2.775	20.477	1.00	17.40
	ATOM	3111	CG2	ILE	B	452	7.464	2.496	19.831	1.00	14.33
	ATOM	3112	CG1	ILE	B	452	9.763	1.635	20.107	1.00	15.36
	ATOM	3113	CD1	ILE	B	452	9.449	0.323	20.805	1.00	17.76
	ATOM	3114	C	ILE	B	452	8.271	5.195	20.024	1.00	17.47
55	ATOM	3115	O	ILE	B	452	7.733	5.586	18.992	1.00	16.50
	ATOM	3116	N	LEU	B	453	7.943	5.665	21.222	1.00	16.06
	ATOM	3117	CA	LEU	B	453	6.903	6.680	21.374	1.00	17.17
	ATOM	3118	CB	LEU	B	453	6.736	7.061	22.850	1.00	16.23
	ATOM	3119	CG	LEU	B	453	5.792	8.228	23.163	1.00	17.60
60	ATOM	3120	CD1	LEU	B	453	4.388	7.881	22.704	1.00	16.94
	ATOM	3121	CD2	LEU	B	453	5.816	8.538	24.667	1.00	17.17

5	ATOM	3122	C	LEU	B	453	7.198	7.941	20.566	1.00	19.33
	ATOM	3123	O	LEU	B	453	6.320	8.458	19.879	1.00	21.37
	ATOM	3124	N	LEU	B	454	8.434	8.428	20.636	1.00	17.68
	ATOM	3125	CA	LEU	B	454	8.789	9.653	19.933	1.00	20.93
10	ATOM	3126	CB	LEU	B	454	9.959	10.347	20.653	1.00	24.33
	ATOM	3127	CG	LEU	B	454	9.735	10.699	22.130	1.00	26.16
	ATOM	3128	CD1	LEU	B	454	11.046	11.170	22.749	1.00	24.82
	ATOM	3129	CD2	LEU	B	454	8.658	11.777	22.259	1.00	23.79
15	ATOM	3130	C	LEU	B	454	9.120	9.494	18.449	1.00	20.75
	ATOM	3131	O	LEU	B	454	8.941	10.431	17.673	1.00	21.33
	ATOM	3132	N	ASN	B	455	9.566	8.311	18.042	1.00	20.54
	ATOM	3133	CA	ASN	B	455	9.951	8.093	16.651	1.00	19.46
20	ATOM	3134	CB	ASN	B	455	11.147	7.149	16.584	1.00	18.58
	ATOM	3135	CG	ASN	B	455	11.576	6.871	15.161	1.00	17.64
	ATOM	3136	OD1	ASN	B	455	12.106	7.749	14.496	1.00	18.40
	ATOM	3137	ND2	ASN	B	455	11.343	5.648	14.686	1.00	15.06
25	ATOM	3138	C	ASN	B	455	8.925	7.580	15.655	1.00	22.77
	ATOM	3139	O	ASN	B	455	8.790	8.127	14.564	1.00	21.94
	ATOM	3140	N	SER	B	456	8.224	6.514	16.023	1.00	25.90
	ATOM	3141	CA	SER	B	456	7.260	5.873	15.135	1.00	24.76
30	ATOM	3142	CB	SER	B	456	6.402	4.894	15.939	1.00	26.91
	ATOM	3143	OG	SER	B	456	7.212	3.818	16.390	1.00	26.24
	ATOM	3144	C	SER	B	456	6.385	6.774	14.272	1.00	26.52
	ATOM	3145	O	SER	B	456	6.323	6.588	13.055	1.00	29.22
35	ATOM	3146	N	GLY	B	457	5.716	7.750	14.872	1.00	22.07
	ATOM	3147	CA	GLY	B	457	4.879	8.627	14.076	1.00	25.19
	ATOM	3148	C	GLY	B	457	5.510	9.973	13.765	1.00	28.59
	ATOM	3149	O	GLY	B	457	4.851	10.850	13.214	1.00	28.31
40	ATOM	3150	N	VAL	B	458	6.789	10.130	14.092	1.00	31.65
	ATOM	3151	CA	VAL	B	458	7.486	11.396	13.879	1.00	38.50
	ATOM	3152	CB	VAL	B	458	8.950	11.310	14.373	1.00	36.24
	ATOM	3153	CG1	VAL	B	458	9.827	10.650	13.324	1.00	38.50
45	ATOM	3154	CG2	VAL	B	458	9.463	12.699	14.701	1.00	39.84
	ATOM	3155	C	VAL	B	458	7.483	11.982	12.464	1.00	46.30
	ATOM	3156	O	VAL	B	458	7.567	13.201	12.302	1.00	47.67
	ATOM	3157	N	TYR	B	459	7.393	11.138	11.442	1.00	50.45
50	ATOM	3158	CA	TYR	B	459	7.385	11.640	10.069	1.00	57.07
	ATOM	3159	CB	TYR	B	459	8.233	10.740	9.170	1.00	57.05
	ATOM	3160	CG	TYR	B	459	9.673	10.680	9.611	1.00	59.29
	ATOM	3161	CD1	TYR	B	459	10.284	11.786	10.203	1.00	60.93
55	ATOM	3162	CE1	TYR	B	459	11.591	11.725	10.662	1.00	61.86
	ATOM	3163	CD2	TYR	B	459	10.414	9.510	9.486	1.00	59.46
	ATOM	3164	CE2	TYR	B	459	11.726	9.439	9.943	1.00	59.67
	ATOM	3165	CZ	TYR	B	459	12.305	10.548	10.532	1.00	60.84
60	ATOM	3166	OH	TYR	B	459	13.593	10.477	11.009	1.00	61.39
	ATOM	3167	C	TYR	B	459	5.976	11.753	9.514	1.00	61.22
	ATOM	3168	O	TYR	B	459	5.629	12.750	8.874	1.00	62.89
	ATOM	3169	N	THR	B	460	5.166	10.730	9.768	1.00	65.15
55	ATOM	3170	CA	THR	B	460	3.783	10.702	9.309	1.00	67.76
	ATOM	3171	CB	THR	B	460	3.178	9.283	9.464	1.00	68.02
	ATOM	3172	OG1	THR	B	460	1.890	9.235	8.836	1.00	67.03
	ATOM	3173	CG2	THR	B	460	3.040	8.916	10.938	1.00	67.31
60	ATOM	3174	C	THR	B	460	2.945	11.700	10.107	1.00	70.14
	ATOM	3175	O	THR	B	460	1.715	11.641	10.099	1.00	72.35
	ATOM	3176	N	PHE	B	461	3.625	12.620	10.788	1.00	72.64
	ATOM	3177	CA	PHE	B	461	2.969	13.637	11.607	1.00	75.05
	ATOM	3178	CB	PHE	B	461	3.977	14.720	12.012	1.00	75.47

5	ATOM	3179	CG	PHE	B	461	4.235	14.789	13.492	1.00	74.32
	ATOM	3180	CD1	PHE	B	461	3.200	14.609	14.404	1.00	73.98
	ATOM	3181	CD2	PHE	B	461	5.517	15.025	13.975	1.00	75.22
	ATOM	3182	CE1	PHE	B	461	3.438	14.662	15.775	1.00	74.02
	ATOM	3183	CE2	PHE	B	461	5.765	15.080	15.344	1.00	74.50
10	ATOM	3184	CZ	PHE	B	461	4.722	14.897	16.245	1.00	74.10
	ATOM	3185	C	PHE	B	461	1.787	14.286	10.896	1.00	76.78
	ATOM	3186	O	PHE	B	461	1.775	14.279	9.645	1.00	77.08
	ATOM	3187	CB	GLU	B	470	7.873	23.789	14.718	1.00	80.19
	ATOM	3188	C	GLU	B	470	8.958	21.731	15.650	1.00	79.30
15	ATOM	3189	O	GLU	B	470	9.887	21.518	16.432	1.00	78.21
	ATOM	3190	N	GLU	B	470	9.096	22.235	13.227	1.00	80.22
	ATOM	3191	CA	GLU	B	470	9.060	22.830	14.595	1.00	80.03
	ATOM	3192	N	GLU	B	471	7.823	21.037	15.665	1.00	78.31
	ATOM	3193	CA	GLU	B	471	7.596	19.956	16.617	1.00	75.83
20	ATOM	3194	CB	GLU	B	471	6.118	19.543	16.604	1.00	76.70
	ATOM	3195	CG	GLU	B	471	5.742	18.544	15.516	1.00	78.42
	ATOM	3196	CD	GLU	B	471	5.062	19.198	14.327	1.00	79.69
	ATOM	3197	OE1	GLU	B	471	3.829	19.398	14.378	1.00	80.26
	ATOM	3198	OE2	GLU	B	471	5.763	19.511	13.340	1.00	80.72
25	ATOM	3199	C	GLU	B	471	8.487	18.756	16.292	1.00	73.13
	ATOM	3200	O	GLU	B	471	8.897	18.021	17.189	1.00	73.86
	ATOM	3201	N	LYS	B	472	8.785	18.565	15.009	1.00	69.65
	ATOM	3202	CA	LYS	B	472	9.639	17.461	14.581	1.00	64.40
	ATOM	3203	CB	LYS	B	472	9.578	17.293	13.060	1.00	63.78
30	ATOM	3204	CG	LYS	B	472	8.343	16.552	12.566	1.00	64.49
	ATOM	3205	CD	LYS	B	472	8.544	16.002	11.161	1.00	63.81
	ATOM	3206	CE	LYS	B	472	7.379	16.368	10.249	1.00	64.90
	ATOM	3207	NZ	LYS	B	472	6.475	15.212	9.990	1.00	63.97
	ATOM	3208	C	LYS	B	472	11.071	17.749	15.014	1.00	61.03
35	ATOM	3209	O	LYS	B	472	11.848	16.833	15.287	1.00	60.28
	ATOM	3210	N	ASP	B	473	11.413	19.033	15.076	1.00	56.84
	ATOM	3211	CA	ASP	B	473	12.745	19.451	15.488	1.00	51.69
	ATOM	3212	CB	ASP	B	473	12.923	20.940	15.242	1.00	50.36
	ATOM	3213	C	ASP	B	473	12.923	19.138	16.970	1.00	49.18
40	ATOM	3214	O	ASP	B	473	13.959	18.619	17.385	1.00	46.85
	ATOM	3215	N	HIS	B	474	11.898	19.449	17.758	1.00	45.35
	ATOM	3216	CA	HIS	B	474	11.923	19.203	19.196	1.00	43.65
	ATOM	3217	CB	HIS	B	474	10.652	19.761	19.847	1.00	43.70
	ATOM	3218	CG	HIS	B	474	10.458	19.326	21.267	1.00	43.86
45	ATOM	3219	CD2	HIS	B	474	11.095	19.688	22.406	1.00	44.12
	ATOM	3220	ND1	HIS	B	474	9.510	18.395	21.638	1.00	46.60
	ATOM	3221	CE1	HIS	B	474	9.572	18.202	22.943	1.00	45.29
	ATOM	3222	NE2	HIS	B	474	10.526	18.975	23.434	1.00	47.96
	ATOM	3223	C	HIS	B	474	12.030	17.707	19.471	1.00	42.38
50	ATOM	3224	O	HIS	B	474	12.834	17.273	20.298	1.00	42.83
	ATOM	3225	N	ILE	B	475	11.214	16.923	18.773	1.00	38.86
	ATOM	3226	CA	ILE	B	475	11.222	15.475	18.943	1.00	36.53
	ATOM	3227	CB	ILE	B	475	10.105	14.822	18.110	1.00	36.56
	ATOM	3228	CG2	ILE	B	475	10.390	13.335	17.911	1.00	36.17
55	ATOM	3229	CG1	ILE	B	475	8.770	14.998	18.832	1.00	35.81
	ATOM	3230	CD1	ILE	B	475	7.598	14.410	18.094	1.00	41.77
	ATOM	3231	C	ILE	B	475	12.575	14.898	18.532	1.00	33.72
	ATOM	3232	O	ILE	B	475	13.112	14.023	19.207	1.00	31.50
	ATOM	3233	N	HIS	B	476	13.121	15.375	17.429	1.00	33.65
60	ATOM	3234	CA	HIS	B	476	14.421	14.886	16.992	1.00	33.31
	ATOM	3235	CB	HIS	B	476	14.782	15.481	15.637	1.00	37.30

5	ATOM	3236	CG	HIS	B	476	14.132	14.781	14.486	1.00	43.64
	ATOM	3237	CD2	HIS	B	476	13.723	13.498	14.342	1.00	45.25
	ATOM	3238	ND1	HIS	B	476	13.816	15.419	13.306	1.00	48.37
	ATOM	3239	CE1	HIS	B	476	13.238	14.560	12.484	1.00	48.87
	ATOM	3240	NE2	HIS	B	476	13.170	13.387	13.089	1.00	48.11
10	ATOM	3241	C	HIS	B	476	15.506	15.213	18.022	1.00	31.20
	ATOM	3242	O	HIS	B	476	16.442	14.436	18.208	1.00	27.25
	ATOM	3243	N	ARG	B	477	15.387	16.365	18.684	1.00	30.64
	ATOM	3244	CA	ARG	B	477	16.361	16.754	19.703	1.00	30.09
	ATOM	3245	CB	ARG	B	477	16.144	18.214	20.121	1.00	33.46
15	ATOM	3246	CG	ARG	B	477	16.322	19.212	18.982	1.00	40.74
	ATOM	3247	CD	ARG	B	477	16.274	20.649	19.479	1.00	45.91
	ATOM	3248	NE	ARG	B	477	17.514	21.020	20.155	1.00	51.37
	ATOM	3249	CZ	ARG	B	477	18.375	21.927	19.702	1.00	53.68
	ATOM	3250	NH1	ARG	B	477	18.140	22.567	18.560	1.00	53.04
20	ATOM	3251	NH2	ARG	B	477	19.480	22.185	20.389	1.00	51.79
	ATOM	3252	C	ARG	B	477	16.232	15.835	20.925	1.00	26.97
	ATOM	3253	O	ARG	B	477	17.233	15.387	21.486	1.00	27.34
	ATOM	3254	N	VAL	B	478	14.999	15.558	21.338	1.00	23.70
	ATOM	3255	CA	VAL	B	478	14.780	14.685	22.482	1.00	24.79
25	ATOM	3256	CB	VAL	B	478	13.286	14.613	22.861	1.00	24.83
	ATOM	3257	CG1	VAL	B	478	13.088	13.646	24.022	1.00	26.23
	ATOM	3258	CG2	VAL	B	478	12.781	15.996	23.243	1.00	28.26
	ATOM	3259	C	VAL	B	478	15.284	13.294	22.112	1.00	26.10
	ATOM	3260	O	VAL	B	478	15.919	12.613	22.927	1.00	24.28
30	ATOM	3261	N	LEU	B	479	15.021	12.889	20.870	1.00	22.92
	ATOM	3262	CA	LEU	B	479	15.456	11.584	20.379	1.00	21.96
	ATOM	3263	CB	LEU	B	479	14.992	11.372	18.930	1.00	22.63
	ATOM	3264	CG	LEU	B	479	13.575	10.798	18.756	1.00	20.82
	ATOM	3265	CD1	LEU	B	479	13.231	10.689	17.274	1.00	22.53
35	ATOM	3266	CD2	LEU	B	479	13.495	9.440	19.420	1.00	23.08
	ATOM	3267	C	LEU	B	479	16.975	11.471	20.453	1.00	21.90
	ATOM	3268	O	LEU	B	479	17.506	10.416	20.778	1.00	23.11
	ATOM	3269	N	ASP	B	480	17.675	12.560	20.143	1.00	23.65
	ATOM	3270	CA	ASP	B	480	19.141	12.566	20.198	1.00	24.29
40	ATOM	3271	CB	ASP	B	480	19.692	13.889	19.649	1.00	26.88
	ATOM	3272	CG	ASP	B	480	19.773	13.914	18.129	1.00	33.32
	ATOM	3273	OD1	ASP	B	480	19.857	12.836	17.499	1.00	35.44
	ATOM	3274	OD2	ASP	B	480	19.757	15.022	17.563	1.00	32.44
	ATOM	3275	C	ASP	B	480	19.590	12.406	21.656	1.00	24.13
45	ATOM	3276	O	ASP	B	480	20.551	11.697	21.956	1.00	24.88
	ATOM	3277	N	LYS	B	481	18.887	13.077	22.560	1.00	25.18
	ATOM	3278	CA	LYS	B	481	19.213	13.010	23.980	1.00	26.78
	ATOM	3279	CB	LYS	B	481	18.262	13.898	24.785	1.00	31.37
	ATOM	3280	CG	LYS	B	481	18.962	14.788	25.804	1.00	43.84
50	ATOM	3281	CD	LYS	B	481	18.780	14.260	27.219	1.00	46.08
	ATOM	3282	CE	LYS	B	481	20.120	13.928	27.865	1.00	50.99
	ATOM	3283	NZ	LYS	B	481	21.177	14.922	27.511	1.00	54.35
	ATOM	3284	C	LYS	B	481	19.124	11.575	24.495	1.00	26.87
	ATOM	3285	O	LYS	B	481	19.951	11.145	25.305	1.00	20.37
55	ATOM	3286	N	ILE	B	482	18.124	10.830	24.027	1.00	23.26
	ATOM	3287	CA	ILE	B	482	17.981	9.452	24.472	1.00	21.07
	ATOM	3288	CB	ILE	B	482	16.655	8.828	24.015	1.00	19.80
	ATOM	3289	CG2	ILE	B	482	16.580	7.370	24.491	1.00	17.40
	ATOM	3290	CG1	ILE	B	482	15.479	9.606	24.602	1.00	17.16
60	ATOM	3291	CD1	ILE	B	482	14.136	9.209	23.991	1.00	19.43
	ATOM	3292	C	ILE	B	482	19.135	8.616	23.947	1.00	20.21

5	ATOM	3293	O	ILE	B	482	19.621	7.722	24.640	1.00	25.55
	ATOM	3294	N	THR	B	483	19.569	8.896	22.722	1.00	21.89
	ATOM	3295	CA	THR	B	483	20.701	8.176	22.141	1.00	22.67
	ATOM	3296	CB	THR	B	483	21.030	8.662	20.695	1.00	23.34
	ATOM	3297	OG1	THR	B	483	19.890	8.475	19.851	1.00	27.33
10	ATOM	3298	CG2	THR	B	483	22.203	7.882	20.116	1.00	24.46
	ATOM	3299	C	THR	B	483	21.913	8.441	23.035	1.00	23.51
	ATOM	3300	O	THR	B	483	22.650	7.520	23.381	1.00	27.01
	ATOM	3301	N	ASP	B	484	22.119	9.703	23.404	1.00	22.88
	ATOM	3302	CA	ASP	B	484	23.237	10.058	24.276	1.00	24.93
15	ATOM	3303	CB	ASP	B	484	23.201	11.546	24.652	1.00	28.69
	ATOM	3304	CG	ASP	B	484	23.504	12.464	23.485	1.00	29.19
	ATOM	3305	OD1	ASP	B	484	23.982	11.984	22.437	1.00	29.63
	ATOM	3306	OD2	ASP	B	484	23.256	13.681	23.627	1.00	32.02
	ATOM	3307	C	ASP	B	484	23.125	9.249	25.567	1.00	24.40
20	ATOM	3308	O	ASP	B	484	24.125	8.780	26.103	1.00	25.60
	ATOM	3309	N	THR	B	485	21.899	9.096	26.066	1.00	20.16
	ATOM	3310	CA	THR	B	485	21.670	8.365	27.307	1.00	22.28
	ATOM	3311	CB	THR	B	485	20.203	8.521	27.763	1.00	24.64
	ATOM	3312	OG1	THR	B	485	19.878	9.914	27.830	1.00	24.28
25	ATOM	3313	CG2	THR	B	485	19.993	7.896	29.133	1.00	23.32
	ATOM	3314	C	THR	B	485	22.017	6.881	27.188	1.00	22.13
	ATOM	3315	O	THR	B	485	22.574	6.284	28.115	1.00	23.30
	ATOM	3316	N	LEU	B	486	21.686	6.290	26.045	1.00	23.08
	ATOM	3317	CA	LEU	B	486	21.969	4.881	25.792	1.00	22.26
30	ATOM	3318	CB	LEU	B	486	21.346	4.452	24.464	1.00	20.93
	ATOM	3319	CG	LEU	B	486	19.878	4.031	24.533	1.00	24.92
	ATOM	3320	CD1	LEU	B	486	19.295	4.003	23.123	1.00	21.96
	ATOM	3321	CD2	LEU	B	486	19.763	2.658	25.196	1.00	23.90
	ATOM	3322	C	LEU	B	486	23.477	4.634	25.742	1.00	24.12
35	ATOM	3323	O	LEU	B	486	23.984	3.681	26.334	1.00	24.02
	ATOM	3324	N	ILE	B	487	24.191	5.490	25.022	1.00	24.53
	ATOM	3325	CA	ILE	B	487	25.640	5.345	24.913	1.00	25.16
	ATOM	3326	CB	ILE	B	487	26.207	6.379	23.899	1.00	25.57
	ATOM	3327	CG2	ILE	B	487	27.725	6.522	24.051	1.00	24.54
40	ATOM	3328	CG1	ILE	B	487	25.857	5.936	22.470	1.00	25.63
	ATOM	3329	CD1	ILE	B	487	26.538	4.646	22.021	1.00	25.68
	ATOM	3330	C	ILE	B	487	26.275	5.518	26.307	1.00	23.60
	ATOM	3331	O	ILE	B	487	27.200	4.794	26.671	1.00	23.65
	ATOM	3332	N	HIS	B	488	25.755	6.456	27.081	1.00	21.75
45	ATOM	3333	CA	HIS	B	488	26.251	6.720	28.431	1.00	26.07
	ATOM	3334	CB	HIS	B	488	25.450	7.871	29.041	1.00	26.99
	ATOM	3335	CG	HIS	B	488	25.818	8.196	30.455	1.00	33.06
	ATOM	3336	CD2	HIS	B	488	25.245	7.838	31.629	1.00	32.79
	ATOM	3337	ND1	HIS	B	488	26.869	9.025	30.779	1.00	36.45
50	ATOM	3338	CE1	HIS	B	488	26.927	9.164	32.091	1.00	35.93
	ATOM	3339	NE2	HIS	B	488	25.953	8.453	32.630	1.00	33.88
	ATOM	3340	C	HIS	B	488	26.123	5.463	29.292	1.00	26.85
	ATOM	3341	O	HIS	B	488	27.071	5.054	29.967	1.00	28.52
	ATOM	3342	N	LEU	B	489	24.949	4.850	29.266	1.00	28.00
55	ATOM	3343	CA	LEU	B	489	24.715	3.642	30.040	1.00	25.94
	ATOM	3344	CB	LEU	B	489	23.298	3.127	29.788	1.00	27.07
	ATOM	3345	CG	LEU	B	489	22.158	3.909	30.445	1.00	31.71
	ATOM	3346	CD1	LEU	B	489	20.827	3.516	29.799	1.00	28.08
	ATOM	3347	CD2	LEU	B	489	22.143	3.616	31.949	1.00	29.30
60	ATOM	3348	C	LEU	B	489	25.718	2.561	29.642	1.00	26.84
	ATOM	3349	O	LEU	B	489	26.241	1.832	30.486	1.00	20.86

5	ATOM	3350	N	MET	B	490	25.978	2.453	28.345	1.00	23.82
	ATOM	3351	CA	MET	B	490	26.900	1.438	27.857	1.00	26.38
	ATOM	3352	CB	MET	B	490	26.775	1.306	26.336	1.00	27.29
	ATOM	3353	CG	MET	B	490	25.418	0.776	25.895	1.00	21.68
	ATOM	3354	SD	MET	B	490	25.208	0.739	24.106	1.00	26.30
10	ATOM	3355	CE	MET	B	490	23.461	0.412	24.022	1.00	19.66
	ATOM	3356	C	MET	B	490	28.341	1.743	28.247	1.00	26.42
	ATOM	3357	O	MET	B	490	29.109	0.833	28.574	1.00	24.76
	ATOM	3358	N	ALA	B	491	28.713	3.018	28.207	1.00	26.67
	ATOM	3359	CA	ALA	B	491	30.074	3.394	28.577	1.00	30.73
15	ATOM	3360	CB	ALA	B	491	30.299	4.882	28.335	1.00	26.66
	ATOM	3361	C	ALA	B	491	30.250	3.053	30.056	1.00	32.08
	ATOM	3362	O	ALA	B	491	31.194	2.361	30.438	1.00	34.66
	ATOM	3363	N	LYS	B	492	29.316	3.523	30.878	1.00	33.17
	ATOM	3364	CA	LYS	B	492	29.354	3.267	32.309	1.00	32.82
20	ATOM	3365	CB	LYS	B	492	28.110	3.849	32.976	1.00	36.38
	ATOM	3366	CG	LYS	B	492	28.412	4.797	34.123	1.00	38.68
	ATOM	3367	CD	LYS	B	492	27.242	4.887	35.084	1.00	41.41
	ATOM	3368	CE	LYS	B	492	26.299	6.013	34.698	1.00	47.57
	ATOM	3369	NZ	LYS	B	492	26.395	7.184	35.618	1.00	50.76
25	ATOM	3370	C	LYS	B	492	29.453	1.771	32.619	1.00	34.08
	ATOM	3371	O	LYS	B	492	30.090	1.382	33.593	1.00	34.31
	ATOM	3372	N	ALA	B	493	28.835	0.935	31.788	1.00	32.03
	ATOM	3373	CA	ALA	B	493	28.867	-0.510	31.998	1.00	30.70
	ATOM	3374	CB	ALA	B	493	27.719	-1.181	31.245	1.00	28.80
30	ATOM	3375	C	ALA	B	493	30.201	-1.156	31.606	1.00	33.75
	ATOM	3376	O	ALA	B	493	30.402	-2.356	31.819	1.00	30.53
	ATOM	3377	N	GLY	B	494	31.102	-0.372	31.020	1.00	33.50
	ATOM	3378	CA	GLY	B	494	32.405	-0.903	30.656	1.00	33.71
	ATOM	3379	C	GLY	B	494	32.639	-1.360	29.230	1.00	34.40
35	ATOM	3380	O	GLY	B	494	33.663	-1.989	28.950	1.00	33.13
	ATOM	3381	N	LEU	B	495	31.712	-1.056	28.326	1.00	31.76
	ATOM	3382	CA	LEU	B	495	31.859	-1.452	26.925	1.00	30.57
	ATOM	3383	CB	LEU	B	495	30.494	-1.415	26.216	1.00	30.67
	ATOM	3384	CG	LEU	B	495	29.610	-2.675	26.256	1.00	29.59
40	ATOM	3385	CD1	LEU	B	495	29.315	-3.058	27.700	1.00	26.60
	ATOM	3386	CD2	LEU	B	495	28.307	-2.416	25.501	1.00	27.52
	ATOM	3387	C	LEU	B	495	32.829	-0.515	26.202	1.00	30.53
	ATOM	3388	O	LEU	B	495	32.855	0.688	26.468	1.00	28.14
	ATOM	3389	N	THR	B	496	33.628	-1.064	25.291	1.00	28.03
45	ATOM	3390	CA	THR	B	496	34.567	-0.243	24.529	1.00	29.06
	ATOM	3391	CB	THR	B	496	35.511	-1.095	23.665	1.00	29.40
	ATOM	3392	OG1	THR	B	496	34.753	-1.758	22.641	1.00	30.29
	ATOM	3393	CG2	THR	B	496	36.228	-2.122	24.515	1.00	28.12
	ATOM	3394	C	THR	B	496	33.770	0.652	23.590	1.00	30.12
50	ATOM	3395	O	THR	B	496	32.580	0.433	23.380	1.00	29.74
	ATOM	3396	N	LEU	B	497	34.430	1.654	23.018	1.00	30.44
	ATOM	3397	CA	LEU	B	497	33.762	2.567	22.104	1.00	28.54
	ATOM	3398	CB	LEU	B	497	34.768	3.564	21.529	1.00	31.14
	ATOM	3399	CG	LEU	B	497	35.209	4.719	22.434	1.00	33.58
55	ATOM	3400	CD1	LEU	B	497	36.120	5.659	21.652	1.00	31.42
	ATOM	3401	CD2	LEU	B	497	33.992	5.469	22.942	1.00	35.08
	ATOM	3402	C	LEU	B	497	33.095	1.800	20.967	1.00	27.35
	ATOM	3403	O	LEU	B	497	31.967	2.105	20.574	1.00	24.03
	ATOM	3404	N	GLN	B	498	33.798	0.797	20.447	1.00	26.17
60	ATOM	3405	CA	GLN	B	498	33.289	-0.009	19.348	1.00	26.32
	ATOM	3406	CB	GLN	B	498	34.411	-0.876	18.771	1.00	27.25

5	ATOM	3407	CG	GLN	B	498	33.967	-1.796	17.645	1.00	32.67
	ATOM	3408	CD	GLN	B	498	34.965	-2.912	17.374	1.00	38.39
	ATOM	3409	OE1	GLN	B	498	35.737	-3.298	18.254	1.00	36.78
	ATOM	3410	NE2	GLN	B	498	34.953	-3.437	16.153	1.00	33.18
	ATOM	3411	C	GLN	B	498	32.112	-0.888	19.774	1.00	25.70
10	ATOM	3412	O	GLN	B	498	31.167	-1.076	19.009	1.00	25.35
	ATOM	3413	N	GLN	B	499	32.173	-1.434	20.986	1.00	24.01
	ATOM	3414	CA	GLN	B	499	31.093	-2.281	21.487	1.00	25.34
	ATOM	3415	CB	GLN	B	499	31.501	-2.935	22.815	1.00	28.38
	ATOM	3416	CG	GLN	B	499	32.537	-4.056	22.669	1.00	29.13
15	ATOM	3417	CD	GLN	B	499	32.913	-4.687	23.995	1.00	30.80
	ATOM	3418	OE1	GLN	B	499	33.306	-3.997	24.937	1.00	33.62
	ATOM	3419	NE2	GLN	B	499	32.797	-6.004	24.074	1.00	30.64
	ATOM	3420	C	GLN	B	499	29.842	-1.430	21.693	1.00	25.70
	ATOM	3421	O	GLN	B	499	28.715	-1.910	21.554	1.00	26.22
20	ATOM	3422	N	GLN	B	500	30.062	-0.160	22.020	1.00	23.09
	ATOM	3423	CA	GLN	B	500	28.989	0.793	22.256	1.00	23.53
	ATOM	3424	CB	GLN	B	500	29.564	2.107	22.782	1.00	26.17
	ATOM	3425	CG	GLN	B	500	29.958	2.073	24.252	1.00	27.71
	ATOM	3426	CD	GLN	B	500	30.812	3.262	24.641	1.00	29.32
25	ATOM	3427	OE1	GLN	B	500	30.559	4.386	24.207	1.00	28.48
	ATOM	3428	NE2	GLN	B	500	31.831	3.021	25.463	1.00	25.07
	ATOM	3429	C	GLN	B	500	28.151	1.074	21.015	1.00	24.24
	ATOM	3430	O	GLN	B	500	26.923	0.949	21.053	1.00	24.40
	ATOM	3431	N	HIS	B	501	28.790	1.465	19.915	1.00	23.08
30	ATOM	3432	CA	HIS	B	501	28.004	1.739	18.724	1.00	26.92
	ATOM	3433	CB	HIS	B	501	28.791	2.577	17.697	1.00	32.00
	ATOM	3434	CG	HIS	B	501	29.988	1.896	17.105	1.00	36.97
	ATOM	3435	CD2	HIS	B	501	30.122	0.710	16.465	1.00	40.32
	ATOM	3436	ND1	HIS	B	501	31.224	2.505	17.042	1.00	37.88
35	ATOM	3437	CE1	HIS	B	501	32.066	1.724	16.389	1.00	38.81
	ATOM	3438	NE2	HIS	B	501	31.422	0.628	16.028	1.00	41.21
	ATOM	3439	C	HIS	B	501	27.451	0.457	18.123	1.00	25.91
	ATOM	3440	O	HIS	B	501	26.369	0.457	17.531	1.00	20.13
	ATOM	3441	N	GLN	B	502	28.165	-0.648	18.317	1.00	24.94
40	ATOM	3442	CA	GLN	B	502	27.698	-1.926	17.804	1.00	21.88
	ATOM	3443	CB	GLN	B	502	28.785	-2.996	17.953	1.00	24.62
	ATOM	3444	CG	GLN	B	502	29.796	-3.001	16.797	1.00	26.55
	ATOM	3445	CD	GLN	B	502	30.843	-4.109	16.902	1.00	27.06
	ATOM	3446	OE1	GLN	B	502	30.716	-5.033	17.705	1.00	28.49
45	ATOM	3447	NE2	GLN	B	502	31.882	-4.018	16.078	1.00	21.90
	ATOM	3448	C	GLN	B	502	26.428	-2.341	18.554	1.00	22.39
	ATOM	3449	O	GLN	B	502	25.464	-2.807	17.944	1.00	22.24
	ATOM	3450	N	ARG	B	503	26.421	-2.159	19.874	1.00	20.54
	ATOM	3451	CA	ARG	B	503	25.259	-2.523	20.678	1.00	22.04
50	ATOM	3452	CB	ARG	B	503	25.602	-2.519	22.180	1.00	22.51
	ATOM	3453	CG	ARG	B	503	24.451	-3.022	23.077	1.00	23.34
	ATOM	3454	CD	ARG	B	503	24.853	-3.110	24.550	1.00	22.18
	ATOM	3455	NE	ARG	B	503	23.743	-3.546	25.395	1.00	19.62
	ATOM	3456	CZ	ARG	B	503	23.329	-4.807	25.497	1.00	19.88
55	ATOM	3457	NH1	ARG	B	503	23.933	-5.765	24.809	1.00	16.40
	ATOM	3458	NH2	ARG	B	503	22.303	-5.110	26.280	1.00	19.71
	ATOM	3459	C	ARG	B	503	24.102	-1.558	20.409	1.00	19.05
	ATOM	3460	O	ARG	B	503	22.945	-1.968	20.351	1.00	18.87
	ATOM	3461	N	LEU	B	504	24.414	-0.276	20.239	1.00	20.19
60	ATOM	3462	CA	LEU	B	504	23.375	0.714	19.969	1.00	19.33
	ATOM	3463	CB	LEU	B	504	23.972	2.117	19.855	1.00	16.25

5	ATOM	3464	CG	LEU	B	504	22.983	3.173	19.344	1.00	20.35
	ATOM	3465	CD1	LEU	B	504	21.930	3.449	20.427	1.00	17.97
	ATOM	3466	CD2	LEU	B	504	23.729	4.448	18.955	1.00	20.86
	ATOM	3467	C	LEU	B	504	22.659	0.357	18.667	1.00	21.22
	ATOM	3468	O	LEU	B	504	21.433	0.478	18.566	1.00	19.28
10	ATOM	3469	N	ALA	B	505	23.428	-0.085	17.676	1.00	18.55
	ATOM	3470	CA	ALA	B	505	22.859	-0.473	16.396	1.00	18.20
	ATOM	3471	CB	ALA	B	505	23.973	-0.745	15.382	1.00	18.45
	ATOM	3472	C	ALA	B	505	21.986	-1.716	16.562	1.00	19.54
	ATOM	3473	O	ALA	B	505	20.871	-1.774	16.041	1.00	17.63
15	ATOM	3474	N	GLN	B	506	22.497	-2.706	17.293	1.00	20.30
	ATOM	3475	CA	GLN	B	506	21.772	-3.955	17.513	1.00	19.48
	ATOM	3476	CB	GLN	B	506	22.590	-4.893	18.409	1.00	21.75
	ATOM	3477	CG	GLN	B	506	23.798	-5.551	17.727	1.00	20.85
	ATOM	3478	CD	GLN	B	506	24.819	-6.070	18.736	1.00	26.18
20	ATOM	3479	OE1	GLN	B	506	24.564	-6.084	19.943	1.00	21.83
	ATOM	3480	NE2	GLN	B	506	25.977	-6.499	18.245	1.00	25.39
	ATOM	3481	C	GLN	B	506	20.421	-3.672	18.166	1.00	21.39
	ATOM	3482	O	GLN	B	506	19.396	-4.233	17.766	1.00	20.87
	ATOM	3483	N	LEU	B	507	20.433	-2.800	19.171	1.00	19.52
25	ATOM	3484	CA	LEU	B	507	19.219	-2.418	19.884	1.00	23.04
	ATOM	3485	CB	LEU	B	507	19.548	-1.455	21.030	1.00	22.82
	ATOM	3486	CG	LEU	B	507	20.182	-2.011	22.313	1.00	26.12
	ATOM	3487	CD1	LEU	B	507	20.203	-0.916	23.360	1.00	29.33
	ATOM	3488	CD2	LEU	B	507	19.415	-3.213	22.816	1.00	27.80
30	ATOM	3489	C	LEU	B	507	18.212	-1.730	18.971	1.00	22.19
	ATOM	3490	O	LEU	B	507	17.036	-2.070	18.964	1.00	23.00
	ATOM	3491	N	LEU	B	508	18.678	-0.745	18.214	1.00	21.53
	ATOM	3492	CA	LEU	B	508	17.797	0.006	17.332	1.00	20.60
	ATOM	3493	CB	LEU	B	508	18.535	1.236	16.805	1.00	17.57
35	ATOM	3494	CG	LEU	B	508	18.934	2.218	17.913	1.00	17.67
	ATOM	3495	CD1	LEU	B	508	19.566	3.446	17.301	1.00	20.04
	ATOM	3496	CD2	LEU	B	508	17.724	2.611	18.725	1.00	18.49
	ATOM	3497	C	LEU	B	508	17.235	-0.831	16.183	1.00	21.17
	ATOM	3498	O	LEU	B	508	16.118	-0.597	15.728	1.00	21.88
40	ATOM	3499	N	LEU	B	509	18.000	-1.813	15.713	1.00	21.89
	ATOM	3500	CA	LEU	B	509	17.511	-2.657	14.631	1.00	22.81
	ATOM	3501	CB	LEU	B	509	18.603	-3.597	14.145	1.00	22.65
	ATOM	3502	CG	LEU	B	509	19.645	-2.891	13.278	1.00	29.11
	ATOM	3503	CD1	LEU	B	509	20.697	-3.888	12.829	1.00	25.69
45	ATOM	3504	CD2	LEU	B	509	18.965	-2.248	12.082	1.00	27.92
	ATOM	3505	C	LEU	B	509	16.302	-3.462	15.095	1.00	23.32
	ATOM	3506	O	LEU	B	509	15.409	-3.759	14.303	1.00	23.36
	ATOM	3507	N	ILE	B	510	16.264	-3.796	16.380	1.00	23.36
	ATOM	3508	CA	ILE	B	510	15.148	-4.562	16.912	1.00	20.99
50	ATOM	3509	CB	ILE	B	510	15.448	-5.041	18.361	1.00	28.60
	ATOM	3510	CG2	ILE	B	510	14.162	-5.435	19.075	1.00	28.10
	ATOM	3511	CG1	ILE	B	510	16.383	-6.260	18.308	1.00	26.57
	ATOM	3512	CD1	ILE	B	510	17.429	-6.301	19.419	1.00	30.14
	ATOM	3513	C	ILE	B	510	13.852	-3.746	16.846	1.00	17.65
55	ATOM	3514	O	ILE	B	510	12.767	-4.308	16.759	1.00	16.11
	ATOM	3515	N	LEU	B	511	13.961	-2.421	16.867	1.00	18.12
	ATOM	3516	CA	LEU	B	511	12.772	-1.574	16.774	1.00	16.95
	ATOM	3517	CB	LEU	B	511	13.147	-0.100	16.981	1.00	22.66
	ATOM	3518	CG	LEU	B	511	13.607	0.262	18.406	1.00	22.13
60	ATOM	3519	CD1	LEU	B	511	13.404	1.751	18.652	1.00	25.29
	ATOM	3520	CD2	LEU	B	511	12.830	-0.549	19.425	1.00	25.08



5	ATOM	3521	C	LEU	B	511	12.112	-1.771	15.397	1.00	16.65
	ATOM	3522	O	LEU	B	511	10.915	-1.578	15.242	1.00	17.09
	ATOM	3523	N	SER	B	512	12.901	-2.161	14.401	1.00	15.83
	ATOM	3524	CA	SER	B	512	12.355	-2.408	13.072	1.00	18.66
	ATOM	3525	CB	SER	B	512	13.484	-2.644	12.074	1.00	17.62
10	ATOM	3526	OG	SER	B	512	13.079	-3.550	11.062	1.00	32.77
	ATOM	3527	C	SER	B	512	11.454	-3.638	13.154	1.00	18.54
	ATOM	3528	O	SER	B	512	10.373	-3.683	12.545	1.00	17.01
	ATOM	3529	N	HIS	B	513	11.899	-4.625	13.929	1.00	15.54
	ATOM	3530	CA	HIS	B	513	11.141	-5.860	14.115	1.00	17.67
15	ATOM	3531	CB	HIS	B	513	12.013	-6.916	14.790	1.00	19.03
	ATOM	3532	CG	HIS	B	513	13.063	-7.475	13.886	1.00	27.06
	ATOM	3533	CD2	HIS	B	513	12.980	-8.364	12.868	1.00	28.40
	ATOM	3534	ND1	HIS	B	513	14.378	-7.066	13.932	1.00	28.92
	ATOM	3535	CE1	HIS	B	513	15.061	-7.678	12.981	1.00	30.75
20	ATOM	3536	NE2	HIS	B	513	14.235	-8.472	12.321	1.00	30.08
	ATOM	3537	C	HIS	B	513	9.895	-5.602	14.958	1.00	15.35
	ATOM	3538	O	HIS	B	513	8.846	-6.192	14.704	1.00	14.83
	ATOM	3539	N	ILE	B	514	10.012	-4.744	15.942	1.00	13.35
	ATOM	3540	CA	ILE	B	514	8.865	-4.417	16.776	1.00	15.48
25	ATOM	3541	CB	ILE	B	514	9.295	-3.534	17.967	1.00	20.02
	ATOM	3542	CG2	ILE	B	514	8.067	-2.918	18.650	1.00	12.84
	ATOM	3543	CG1	ILE	B	514	10.093	-4.397	18.962	1.00	22.87
	ATOM	3544	CD1	ILE	B	514	10.691	-3.641	20.115	1.00	29.62
	ATOM	3545	C	ILE	B	514	7.797	-3.717	15.923	1.00	15.16
30	ATOM	3546	O	ILE	B	514	6.606	-3.972	16.078	1.00	16.61
	ATOM	3547	N	ARG	B	515	8.224	-2.823	15.030	1.00	16.33
	ATOM	3548	CA	ARG	B	515	7.280	-2.138	14.150	1.00	17.54
	ATOM	3549	CB	ARG	B	515	8.010	-1.173	13.214	1.00	20.15
	ATOM	3550	CG	ARG	B	515	7.080	-0.454	12.234	1.00	21.47
35	ATOM	3551	CD	ARG	B	515	6.407	0.749	12.891	1.00	26.05
	ATOM	3552	NE	ARG	B	515	7.220	1.948	12.716	1.00	24.91
	ATOM	3553	CZ	ARG	B	515	6.734	3.175	12.547	1.00	24.61
	ATOM	3554	NH1	ARG	B	515	5.424	3.393	12.522	1.00	22.46
	ATOM	3555	NH2	ARG	B	515	7.569	4.182	12.374	1.00	23.15
40	ATOM	3556	C	ARG	B	515	6.545	-3.182	13.304	1.00	16.60
	ATOM	3557	O	ARG	B	515	5.332	-3.093	13.087	1.00	14.51
	ATOM	3558	N	HIS	B	516	7.298	-4.171	12.827	1.00	18.50
	ATOM	3559	CA	HIS	B	516	6.743	-5.237	11.997	1.00	17.26
	ATOM	3560	CB	HIS	B	516	7.861	-6.176	11.533	1.00	18.14
45	ATOM	3561	CG	HIS	B	516	7.405	-7.223	10.568	1.00	24.87
	ATOM	3562	CD2	HIS	B	516	7.060	-8.521	10.754	1.00	26.64
	ATOM	3563	ND1	HIS	B	516	7.258	-6.978	9.220	1.00	21.82
	ATOM	3564	CE1	HIS	B	516	6.839	-8.078	8.619	1.00	28.42
	ATOM	3565	NE2	HIS	B	516	6.711	-9.028	9.526	1.00	24.47
50	ATOM	3566	C	HIS	B	516	5.685	-6.028	12.759	1.00	16.87
	ATOM	3567	O	HIS	B	516	4.596	-6.303	12.240	1.00	14.81
	ATOM	3568	N	MET	B	517	5.999	-6.396	13.997	1.00	16.48
	ATOM	3569	CA	MET	B	517	5.049	-7.162	14.801	1.00	15.39
	ATOM	3570	CB	MET	B	517	5.701	-7.587	16.114	1.00	21.05
55	ATOM	3571	CG	MET	B	517	6.790	-8.638	15.917	1.00	20.76
	ATOM	3572	SD	MET	B	517	7.380	-9.320	17.470	1.00	23.96
	ATOM	3573	CE	MET	B	517	8.104	-7.879	18.226	1.00	20.45
	ATOM	3574	C	MET	B	517	3.789	-6.368	15.080	1.00	16.23
	ATOM	3575	O	MET	B	517	2.688	-6.924	15.148	1.00	16.02
60	ATOM	3576	N	SER	B	518	3.954	-5.060	15.247	1.00	13.32
	ATOM	3577	CA	SER	B	518	2.827	-4.186	15.505	1.00	16.34

5	ATOM	3578	CB	SER	B	518	3.316	-2.765	15.835	1.00	17.48
	ATOM	3579	OG	SER	B	518	2.234	-1.840	15.843	1.00	17.46
	ATOM	3580	C	SER	B	518	1.906	-4.147	14.284	1.00	14.73
	ATOM	3581	O	SER	B	518	0.688	-4.247	14.417	1.00	19.16
	ATOM	3582	N	ASN	B	519	2.474	-4.006	13.091	1.00	14.52
10	ATOM	3583	CA	ASN	B	519	1.622	-3.953	11.907	1.00	15.35
	ATOM	3584	CB	ASN	B	519	2.432	-3.509	10.698	1.00	19.21
	ATOM	3585	CG	ASN	B	519	2.700	-2.029	10.729	1.00	20.58
	ATOM	3586	OD1	ASN	B	519	1.839	-1.258	11.150	1.00	26.36
	ATOM	3587	ND2	ASN	B	519	3.891	-1.618	10.307	1.00	19.62
15	ATOM	3588	C	ASN	B	519	0.911	-5.280	11.658	1.00	16.74
	ATOM	3589	O	ASN	B	519	-0.265	-5.299	11.297	1.00	20.58
	ATOM	3590	N	LYS	B	520	1.608	-6.387	11.885	1.00	18.60
	ATOM	3591	CA	LYS	B	520	0.992	-7.699	11.717	1.00	20.04
	ATOM	3592	CB	LYS	B	520	2.038	-8.801	11.872	1.00	25.44
20	ATOM	3593	CG	LYS	B	520	3.037	-8.849	10.728	1.00	31.68
	ATOM	3594	CD	LYS	B	520	2.507	-9.663	9.558	1.00	42.56
	ATOM	3595	CE	LYS	B	520	2.186	-8.778	8.364	1.00	45.61
	ATOM	3596	NZ	LYS	B	520	1.435	-9.526	7.312	1.00	46.00
	ATOM	3597	C	LYS	B	520	-0.099	-7.868	12.769	1.00	18.88
25	ATOM	3598	O	LYS	B	520	-1.183	-8.358	12.478	1.00	21.75
	ATOM	3599	N	GLY	B	521	0.191	-7.455	13.998	1.00	17.83
	ATOM	3600	CA	GLY	B	521	-0.792	-7.569	15.058	1.00	16.19
	ATOM	3601	C	GLY	B	521	-2.000	-6.674	14.833	1.00	16.59
	ATOM	3602	O	GLY	B	521	-3.128	-7.060	15.125	1.00	16.57
30	ATOM	3603	N	MET	B	522	-1.766	-5.467	14.326	1.00	17.48
	ATOM	3604	CA	MET	B	522	-2.852	-4.527	14.042	1.00	18.25
	ATOM	3605	CB	MET	B	522	-2.276	-3.212	13.516	1.00	21.27
	ATOM	3606	CG	MET	B	522	-3.190	-2.018	13.707	1.00	26.97
	ATOM	3607	SD	MET	B	522	-3.199	-1.477	15.417	1.00	30.35
35	ATOM	3608	CE	MET	B	522	-1.659	-0.605	15.475	1.00	29.86
	ATOM	3609	C	MET	B	522	-3.794	-5.119	12.989	1.00	18.68
	ATOM	3610	O	MET	B	522	-5.022	-5.008	13.097	1.00	18.80
	ATOM	3611	N	GLU	B	523	-3.205	-5.731	11.966	1.00	18.22
	ATOM	3612	CA	GLU	B	523	-3.968	-6.357	10.889	1.00	23.41
40	ATOM	3613	CB	GLU	B	523	-3.031	-6.946	9.830	1.00	28.74
	ATOM	3614	CG	GLU	B	523	-2.224	-5.935	9.030	1.00	34.42
	ATOM	3615	CD	GLU	B	523	-1.095	-6.597	8.239	1.00	45.58
	ATOM	3616	OE1	GLU	B	523	-0.131	-5.894	7.857	1.00	49.48
	ATOM	3617	OE2	GLU	B	523	-1.169	-7.825	7.999	1.00	45.97
45	ATOM	3618	C	GLU	B	523	-4.812	-7.482	11.465	1.00	23.98
	ATOM	3619	O	GLU	B	523	-5.993	-7.616	11.147	1.00	22.08
	ATOM	3620	N	HIS	B	524	-4.187	-8.287	12.326	1.00	23.46
	ATOM	3621	CA	HIS	B	524	-4.846	-9.428	12.952	1.00	26.20
	ATOM	3622	CB	HIS	B	524	-3.824	-10.245	13.743	1.00	27.26
50	ATOM	3623	CG	HIS	B	524	-4.378	-11.509	14.321	1.00	30.91
	ATOM	3624	CD2	HIS	B	524	-4.308	-12.792	13.892	1.00	30.90
	ATOM	3625	ND1	HIS	B	524	-5.107	-11.537	15.490	1.00	28.87
	ATOM	3626	CE1	HIS	B	524	-5.461	-12.780	15.757	1.00	30.45
	ATOM	3627	NE2	HIS	B	524	-4.989	-13.561	14.803	1.00	29.19
55	ATOM	3628	C	HIS	B	524	-5.996	-9.025	13.870	1.00	27.69
	ATOM	3629	O	HIS	B	524	-7.061	-9.656	13.860	1.00	25.00
	ATOM	3630	N	LEU	B	525	-5.777	-7.977	14.655	1.00	23.84
	ATOM	3631	CA	LEU	B	525	-6.786	-7.492	15.588	1.00	25.77
	ATOM	3632	CB	LEU	B	525	-6.217	-6.358	16.444	1.00	22.22
60	ATOM	3633	CG	LEU	B	525	-7.164	-5.778	17.498	1.00	26.81
	ATOM	3634	CD1	LEU	B	525	-7.763	-6.922	18.321	1.00	23.32

5	ATOM	3635	CD2	LEU	B	525	-6.414	-4.793	18.399	1.00	18.95
	ATOM	3636	C	LEU	B	525	-8.013	-6.995	14.842	1.00	26.84
	ATOM	3637	O	LEU	B	525	-9.154	-7.247	15.249	1.00	26.73
	ATOM	3638	N	TYR	B	526	-7.764	-6.271	13.757	1.00	26.86
	ATOM	3639	CA	TYR	B	526	-8.819	-5.726	12.918	1.00	30.89
10	ATOM	3640	CB	TYR	B	526	-8.201	-4.818	11.854	1.00	34.31
	ATOM	3641	CG	TYR	B	526	-9.183	-4.223	10.878	1.00	43.50
	ATOM	3642	CD1	TYR	B	526	-10.058	-3.211	11.267	1.00	47.66
	ATOM	3643	CE1	TYR	B	526	-10.943	-2.636	10.357	1.00	48.85
	ATOM	3644	CD2	TYR	B	526	-9.218	-4.651	9.552	1.00	48.52
15	ATOM	3645	CE2	TYR	B	526	-10.098	-4.083	8.634	1.00	52.43
	ATOM	3646	CZ	TYR	B	526	-10.955	-3.077	9.043	1.00	51.67
	ATOM	3647	OH	TYR	B	526	-11.810	-2.504	8.129	1.00	57.01
	ATOM	3648	C	TYR	B	526	-9.577	-6.880	12.265	1.00	30.90
	ATOM	3649	O	TYR	B	526	-10.793	-6.829	12.113	1.00	31.48
20	ATOM	3650	N	SER	B	527	-8.849	-7.926	11.889	1.00	31.39
	ATOM	3651	CA	SER	B	527	-9.460	-9.095	11.266	1.00	33.73
	ATOM	3652	CB	SER	B	527	-8.377	-10.048	10.749	1.00	34.13
	ATOM	3653	OG	SER	B	527	-8.945	-11.222	10.196	1.00	43.67
	ATOM	3654	C	SER	B	527	-10.339	-9.813	12.288	1.00	34.34
25	ATOM	3655	O	SER	B	527	-11.446	-10.261	11.973	1.00	33.42
	ATOM	3656	N	MET	B	528	-9.840	-9.916	13.517	1.00	31.66
	ATOM	3657	CA	MET	B	528	-10.574	-10.572	14.589	1.00	29.77
	ATOM	3658	CB	MET	B	528	-9.682	-10.743	15.820	1.00	32.96
	ATOM	3659	CG	MET	B	528	-8.651	-11.859	15.699	1.00	33.47
30	ATOM	3660	SD	MET	B	528	-9.359	-13.427	15.134	1.00	38.28
	ATOM	3661	CE	MET	B	528	-10.265	-13.915	16.579	1.00	36.01
	ATOM	3662	C	MET	B	528	-11.800	-9.747	14.953	1.00	29.42
	ATOM	3663	O	MET	B	528	-12.835	-10.293	15.331	1.00	28.65
	ATOM	3664	N	LYS	B	529	-11.673	-8.429	14.850	1.00	30.64
35	ATOM	3665	CA	LYS	B	529	-12.781	-7.533	15.149	1.00	31.80
	ATOM	3666	CB	LYS	B	529	-12.323	-6.079	15.027	1.00	32.86
	ATOM	3667	CG	LYS	B	529	-13.436	-5.043	15.114	1.00	36.42
	ATOM	3668	CD	LYS	B	529	-13.114	-3.852	14.224	1.00	41.74
	ATOM	3669	CE	LYS	B	529	-13.734	-2.564	14.741	1.00	43.45
40	ATOM	3670	NZ	LYS	B	529	-15.221	-2.569	14.634	1.00	46.51
	ATOM	3671	C	LYS	B	529	-13.857	-7.840	14.116	1.00	36.60
	ATOM	3672	O	LYS	B	529	-15.049	-7.877	14.424	1.00	34.04
	ATOM	3673	N	CYS	B	530	-13.407	-8.083	12.889	1.00	40.04
	ATOM	3674	CA	CYS	B	530	-14.286	-8.409	11.773	1.00	44.58
45	ATOM	3675	CB	CYS	B	530	-13.460	-8.535	10.491	1.00	50.64
	ATOM	3676	SG	CYS	B	530	-13.369	-7.034	9.504	1.00	67.65
	ATOM	3677	C	CYS	B	530	-15.065	-9.692	12.016	1.00	42.88
	ATOM	3678	O	CYS	B	530	-16.274	-9.741	11.807	1.00	40.15
	ATOM	3679	N	LYS	B	531	-14.360	-10.733	12.447	1.00	41.92
50	ATOM	3680	CA	LYS	B	531	-14.980	-12.023	12.728	1.00	42.60
	ATOM	3681	CB	LYS	B	531	-13.907	-13.091	12.927	1.00	44.77
	ATOM	3682	C	LYS	B	531	-15.844	-11.907	13.977	1.00	44.43
	ATOM	3683	O	LYS	B	531	-16.623	-12.804	14.296	1.00	44.09
	ATOM	3684	N	ASN	B	532	-15.678	-10.793	14.685	1.00	44.98
55	ATOM	3685	CA	ASN	B	532	-16.437	-10.496	15.893	1.00	44.10
	ATOM	3686	CB	ASN	B	532	-17.833	-10.003	15.506	1.00	45.14
	ATOM	3687	CG	ASN	B	532	-18.526	-9.271	16.633	1.00	46.54
	ATOM	3688	OD1	ASN	B	532	-19.729	-9.424	16.837	1.00	50.62
	ATOM	3689	ND2	ASN	B	532	-17.771	-8.471	17.375	1.00	46.07
60	ATOM	3690	C	ASN	B	532	-16.557	-11.657	16.882	1.00	43.34
	ATOM	3691	O	ASN	B	532	-17.655	-11.994	17.321	1.00	41.42

5	ATOM	3692	N	VAL	B	533	-15.434	-12.264	17.243	1.00	43.45
	ATOM	3693	CA	VAL	B	533	-15.471	-13.371	18.190	1.00	44.06
	ATOM	3694	CB	VAL	B	533	-14.170	-14.219	18.120	1.00	45.56
	ATOM	3695	CG1	VAL	B	533	-13.661	-14.263	16.683	1.00	45.67
	ATOM	3696	CG2	VAL	B	533	-13.107	-13.644	19.045	1.00	44.16
10	ATOM	3697	C	VAL	B	533	-15.670	-12.835	19.611	1.00	43.24
	ATOM	3698	O	VAL	B	533	-15.894	-13.602	20.548	1.00	44.21
	ATOM	3699	N	VAL	B	534	-15.596	-11.511	19.755	1.00	40.44
	ATOM	3700	CA	VAL	B	534	-15.765	-10.849	21.049	1.00	37.80
	ATOM	3701	CB	VAL	B	534	-14.630	-11.259	22.038	1.00	36.38
15	ATOM	3702	CG1	VAL	B	534	-13.324	-10.575	21.658	1.00	34.35
	ATOM	3703	CG2	VAL	B	534	-15.021	-10.910	23.463	1.00	39.34
	ATOM	3704	C	VAL	B	534	-15.752	-9.329	20.857	1.00	37.97
	ATOM	3705	O	VAL	B	534	-15.026	-8.808	20.008	1.00	39.45
	ATOM	3706	N	PRO	B	535	-16.575	-8.597	21.625	1.00	37.81
20	ATOM	3707	CD	PRO	B	535	-17.529	-9.078	22.640	1.00	38.74
	ATOM	3708	CA	PRO	B	535	-16.608	-7.135	21.492	1.00	36.79
	ATOM	3709	CB	PRO	B	535	-17.846	-6.729	22.288	1.00	36.98
	ATOM	3710	CG	PRO	B	535	-18.004	-7.809	23.298	1.00	39.77
	ATOM	3711	C	PRO	B	535	-15.338	-6.494	22.049	1.00	33.95
25	ATOM	3712	O	PRO	B	535	-14.786	-6.963	23.040	1.00	34.93
	ATOM	3713	N	LEU	B	536	-14.881	-5.426	21.409	1.00	33.42
	ATOM	3714	CA	LEU	B	536	-13.675	-4.732	21.851	1.00	33.40
	ATOM	3715	CB	LEU	B	536	-12.829	-4.314	20.647	1.00	29.31
	ATOM	3716	CG	LEU	B	536	-12.219	-5.433	19.798	1.00	30.06
30	ATOM	3717	CD1	LEU	B	536	-11.344	-4.822	18.714	1.00	30.85
	ATOM	3718	CD2	LEU	B	536	-11.398	-6.370	20.676	1.00	28.96
	ATOM	3719	C	LEU	B	536	-14.036	-3.498	22.666	1.00	30.50
	ATOM	3720	O	LEU	B	536	-15.024	-2.829	22.383	1.00	29.91
	ATOM	3721	N	TYR	B	537	-13.231	-3.194	23.676	1.00	28.69
35	ATOM	3722	CA	TYR	B	537	-13.494	-2.032	24.505	1.00	29.89
	ATOM	3723	CB	TYR	B	537	-12.618	-2.071	25.750	1.00	32.50
	ATOM	3724	CG	TYR	B	537	-12.849	-3.327	26.543	1.00	39.46
	ATOM	3725	CD1	TYR	B	537	-13.923	-3.431	27.421	1.00	41.90
	ATOM	3726	CE1	TYR	B	537	-14.174	-4.609	28.118	1.00	45.72
40	ATOM	3727	CD2	TYR	B	537	-12.022	-4.435	26.379	1.00	47.39
	ATOM	3728	CE2	TYR	B	537	-12.262	-5.620	27.072	1.00	49.93
	ATOM	3729	CZ	TYR	B	537	-13.340	-5.699	27.940	1.00	48.80
	ATOM	3730	OH	TYR	B	537	-13.582	-6.872	28.624	1.00	53.90
	ATOM	3731	C	TYR	B	537	-13.262	-0.761	23.709	1.00	27.09
45	ATOM	3732	O	TYR	B	537	-12.518	-0.757	22.729	1.00	26.15
	ATOM	3733	N	ASP	B	538	-13.909	0.315	24.141	1.00	26.12
	ATOM	3734	CA	ASP	B	538	-13.830	1.598	23.461	1.00	25.27
	ATOM	3735	CB	ASP	B	538	-14.748	2.598	24.164	1.00	28.85
	ATOM	3736	CG	ASP	B	538	-16.227	2.285	23.940	1.00	33.90
50	ATOM	3737	OD1	ASP	B	538	-17.052	2.613	24.819	1.00	32.68
	ATOM	3738	OD2	ASP	B	538	-16.562	1.707	22.882	1.00	38.26
	ATOM	3739	C	ASP	B	538	-12.447	2.217	23.261	1.00	25.18
	ATOM	3740	O	ASP	B	538	-12.120	2.626	22.147	1.00	26.41
	ATOM	3741	N	LEU	B	539	-11.637	2.309	24.313	1.00	20.76
55	ATOM	3742	CA	LEU	B	539	-10.312	2.911	24.150	1.00	19.65
	ATOM	3743	CB	LEU	B	539	-9.567	2.991	25.496	1.00	17.48
	ATOM	3744	CG	LEU	B	539	-8.116	3.511	25.469	1.00	16.46
	ATOM	3745	CD1	LEU	B	539	-8.051	4.892	24.838	1.00	16.43
	ATOM	3746	CD2	LEU	B	539	-7.564	3.569	26.895	1.00	15.57
60	ATOM	3747	C	LEU	B	539	-9.484	2.127	23.127	1.00	16.75
	ATOM	3748	O	LEU	B	539	-8.862	2.716	22.249	1.00	20.36

5	ATOM	3749	N	LEU	B	540	-9.487	0.803	23.239	1.00	18.23
	ATOM	3750	CA	LEU	B	540	-8.743	-0.048	22.319	1.00	18.05
	ATOM	3751	CB	LEU	B	540	-8.909	-1.528	22.701	1.00	16.38
	ATOM	3752	CG	LEU	B	540	-8.188	-2.554	21.821	1.00	19.81
	ATOM	3753	CD1	LEU	B	540	-6.679	-2.303	21.828	1.00	19.27
10	ATOM	3754	CD2	LEU	B	540	-8.473	-3.952	22.327	1.00	18.00
	ATOM	3755	C	LEU	B	540	-9.241	0.169	20.891	1.00	21.50
	ATOM	3756	O	LEU	B	540	-8.449	0.293	19.964	1.00	20.41
	ATOM	3757	N	LEU	B	541	-10.559	0.206	20.726	1.00	22.40
	ATOM	3758	CA	LEU	B	541	-11.164	0.419	19.413	1.00	23.27
15	ATOM	3759	CB	LEU	B	541	-12.686	0.429	19.527	1.00	25.12
	ATOM	3760	CG	LEU	B	541	-13.410	-0.808	18.999	1.00	36.53
	ATOM	3761	CD1	LEU	B	541	-14.910	-0.671	19.273	1.00	30.98
	ATOM	3762	CD2	LEU	B	541	-13.136	-0.971	17.508	1.00	31.93
	ATOM	3763	C	LEU	B	541	-10.697	1.751	18.842	1.00	22.46
20	ATOM	3764	O	LEU	B	541	-10.359	1.845	17.666	1.00	26.29
	ATOM	3765	N	GLU	B	542	-10.694	2.781	19.680	1.00	23.96
	ATOM	3766	CA	GLU	B	542	-10.248	4.106	19.270	1.00	26.91
	ATOM	3767	CB	GLU	B	542	-10.250	5.050	20.468	1.00	30.84
	ATOM	3768	CG	GLU	B	542	-11.166	6.245	20.347	1.00	37.20
25	ATOM	3769	CD	GLU	B	542	-11.138	7.105	21.597	1.00	39.98
	ATOM	3770	OE1	GLU	B	542	-12.223	7.385	22.144	1.00	39.92
	ATOM	3771	OE2	GLU	B	542	-10.028	7.494	22.034	1.00	38.96
	ATOM	3772	C	GLU	B	542	-8.826	4.010	18.724	1.00	27.90
	ATOM	3773	O	GLU	B	542	-8.530	4.492	17.634	1.00	29.32
30	ATOM	3774	N	MET	B	543	-7.945	3.388	19.499	1.00	26.41
	ATOM	3775	CA	MET	B	543	-6.552	3.237	19.107	1.00	23.53
	ATOM	3776	CB	MET	B	543	-5.749	2.591	20.247	1.00	24.60
	ATOM	3777	CG	MET	B	543	-5.812	3.338	21.579	1.00	26.46
	ATOM	3778	SD	MET	B	543	-5.373	5.084	21.467	1.00	29.45
35	ATOM	3779	CE	MET	B	543	-3.585	4.971	21.349	1.00	25.43
	ATOM	3780	C	MET	B	543	-6.403	2.407	17.832	1.00	25.80
	ATOM	3781	O	MET	B	543	-5.535	2.686	17.004	1.00	23.59
	ATOM	3782	N	LEU	B	544	-7.254	1.394	17.673	1.00	27.74
	ATOM	3783	CA	LEU	B	544	-7.202	0.522	16.499	1.00	26.32
40	ATOM	3784	CB	LEU	B	544	-8.069	-0.721	16.719	1.00	26.75
	ATOM	3785	CG	LEU	B	544	-8.274	-1.632	15.502	1.00	28.12
	ATOM	3786	CD1	LEU	B	544	-6.956	-2.294	15.136	1.00	26.36
	ATOM	3787	CD2	LEU	B	544	-9.330	-2.680	15.803	1.00	27.00
	ATOM	3788	C	LEU	B	544	-7.672	1.252	15.250	1.00	26.97
45	ATOM	3789	O	LEU	B	544	-7.036	1.181	14.195	1.00	24.25
	ATOM	3790	N	ASP	B	545	-8.787	1.961	15.372	1.00	30.37
	ATOM	3791	CA	ASP	B	545	-9.338	2.702	14.244	1.00	32.34
	ATOM	3792	CB	ASP	B	545	-10.668	3.346	14.637	1.00	36.61
	ATOM	3793	CG	ASP	B	545	-11.818	2.370	14.565	1.00	42.73
50	ATOM	3794	OD1	ASP	B	545	-12.858	2.624	15.211	1.00	47.39
	ATOM	3795	OD2	ASP	B	545	-11.676	1.342	13.863	1.00	46.96
	ATOM	3796	C	ASP	B	545	-8.382	3.762	13.711	1.00	31.27
	ATOM	3797	O	ASP	B	545	-8.443	4.120	12.532	1.00	30.53
	ATOM	3798	N	ALA	B	546	-7.506	4.272	14.572	1.00	29.02
55	ATOM	3799	CA	ALA	B	546	-6.543	5.280	14.141	1.00	31.21
	ATOM	3800	CB	ALA	B	546	-5.646	5.693	15.306	1.00	30.98
	ATOM	3801	C	ALA	B	546	-5.697	4.731	12.996	1.00	32.14
	ATOM	3802	O	ALA	B	546	-5.189	5.490	12.170	1.00	33.78
	ATOM	3803	N	HIS	B	547	-5.555	3.410	12.943	1.00	32.27
60	ATOM	3804	CA	HIS	B	547	-4.773	2.767	11.892	1.00	37.73
	ATOM	3805	CB	HIS	B	547	-3.991	1.576	12.457	1.00	35.83

5	ATOM	3806	CG	HIS	B	547	-2.796	1.968	13.269	1.00	34.54
	ATOM	3807	CD2	HIS	B	547	-2.698	2.553	14.486	1.00	30.23
	ATOM	3808	ND1	HIS	B	547	-1.502	1.755	12.840	1.00	34.23
	ATOM	3809	CE1	HIS	B	547	-0.659	2.193	13.760	1.00	36.72
	ATOM	3810	NE2	HIS	B	547	-1.360	2.681	14.768	1.00	31.48
10	ATOM	3811	C	HIS	B	547	-5.649	2.286	10.735	1.00	43.69
	ATOM	3812	O	HIS	B	547	-5.178	2.152	9.606	1.00	46.04
	ATOM	3813	N	ARG	B	548	-6.919	2.020	11.019	1.00	48.35
	ATOM	3814	CA	ARG	B	548	-7.843	1.551	9.993	1.00	54.74
	ATOM	3815	CB	ARG	B	548	-8.522	0.267	10.452	1.00	54.66
15	ATOM	3816	C	ARG	B	548	-8.886	2.619	9.681	1.00	59.94
	ATOM	3817	O	ARG	B	548	-8.580	3.812	9.672	1.00	62.81
	ATOM	3818	N	LEU	B	549	-10.116	2.186	9.422	1.00	64.81
	ATOM	3819	CA	LEU	B	549	-11.204	3.109	9.112	1.00	67.59
	ATOM	3820	CB	LEU	B	549	-12.478	2.327	8.799	1.00	68.06
20	ATOM	3821	C	LEU	B	549	-11.449	4.069	10.275	1.00	69.12
	ATOM	3822	O	LEU	B	549	-11.451	5.297	10.036	1.00	68.96
	ATOM	3823	OXT	LEU	B	549	-11.634	3.579	11.412	1.00	70.70
	HETATM	3824	CP9	DES	B	600	-4.547	-6.077	22.000	1.00	18.55
	HETATM	3825	CP8	DES	B	600	-3.163	-6.365	21.467	1.00	17.72
25	HETATM	3826	CP7	DES	B	600	-2.897	-7.853	21.381	1.00	21.17
	HETATM	3827	CP6	DES	B	600	-3.719	-8.551	20.374	1.00	22.05
	HETATM	3828	CP1	DES	B	600	-3.405	-8.481	18.998	1.00	21.32
	HETATM	3829	CP2	DES	B	600	-4.239	-9.095	18.063	1.00	21.61
	HETATM	3830	CP3	DES	B	600	-5.388	-9.771	18.509	1.00	24.89
30	HETATM	3831	OP3	DES	B	600	-6.244	-10.339	17.600	1.00	24.94
	HETATM	3832	CP4	DES	B	600	-5.718	-9.858	19.860	1.00	24.08
	HETATM	3833	CP5	DES	B	600	-4.877	-9.240	20.791	1.00	24.67
	HETATM	3834	C7	DES	B	600	-1.998	-8.460	22.190	1.00	16.67
	HETATM	3835	C6	DES	B	600	-1.330	-7.834	23.325	1.00	15.39
35	HETATM	3836	C5	DES	B	600	-2.054	-7.642	24.522	1.00	17.62
	HETATM	3837	C4	DES	B	600	-1.433	-7.072	25.634	1.00	16.16
	HETATM	3838	C3	DES	B	600	-0.077	-6.685	25.542	1.00	20.04
	HETATM	3839	O3	DES	B	600	0.509	-6.113	26.655	1.00	15.55
	HETATM	3840	C2	DES	B	600	0.669	-6.866	24.353	1.00	18.94
40	HETATM	3841	C1	DES	B	600	0.035	-7.440	23.241	1.00	15.20
	HETATM	3842	C8	DES	B	600	-1.642	-9.903	21.942	1.00	17.61
	HETATM	3843	C9	DES	B	600	-0.440	-10.009	20.998	1.00	11.63
	HETATM	3844	C1	CBM	B	417	-4.997	-22.994	25.273	1.00	55.80
	HETATM	3845	O4	CBM	B	417	-4.789	-24.187	25.003	1.00	55.56
45	HETATM	3846	O3	CBM	B	417	-4.798	-22.559	26.552	1.00	56.04
	HETATM	3847	C2	CBM	B	417	-5.468	-21.960	24.264	1.00	57.04
	HETATM	3848	C1	CBM	B	530	-15.278	-5.124	10.243	1.00	87.39
	HETATM	3849	O4	CBM	B	530	-15.852	-5.086	9.064	1.00	87.68
	HETATM	3850	O3	CBM	B	530	-15.832	-4.291	11.201	1.00	86.22
50	HETATM	3851	C2	CBM	B	530	-14.207	-5.886	10.628	1.00	87.65
	ATOM	3852	CB	HIS	C	687	9.818	-20.030	-2.211	1.00	63.34
	ATOM	3853	C	HIS	C	687	10.133	-20.267	-4.689	1.00	63.49
	ATOM	3854	O	HIS	C	687	11.204	-20.840	-4.472	1.00	63.87
	ATOM	3855	N	HIS	C	687	7.944	-19.563	-3.758	1.00	65.42
55	ATOM	3856	CA	HIS	C	687	9.424	-19.484	-3.586	1.00	64.86
	ATOM	3857	N	LYS	C	688	9.533	-20.281	-5.875	1.00	62.00
	ATOM	3858	CA	LYS	C	688	10.101	-20.999	-7.009	1.00	60.81
	ATOM	3859	CB	LYS	C	688	8.980	-21.540	-7.901	1.00	61.76
	ATOM	3860	C	LYS	C	688	11.050	-20.127	-7.827	1.00	57.47
60	ATOM	3861	O	LYS	C	688	12.253	-20.379	-7.858	1.00	57.64
	ATOM	3862	N	ILE	C	689	10.511	-19.103	-8.482	1.00	55.74

5	ATOM	3863	CA	ILE	C	689	11.326	-18.212	-9.306	1.00	53.09
	ATOM	3864	CB	ILE	C	689	10.496	-17.057	-9.889	1.00	53.83
	ATOM	3865	CG2	ILE	C	689	11.334	-16.286	-10.902	1.00	54.55
	ATOM	3866	CG1	ILE	C	689	9.229	-17.603	-10.551	1.00	52.90
	ATOM	3867	CD1	ILE	C	689	8.406	-16.550	-11.258	1.00	50.45
10	ATOM	3868	C	ILE	C	689	12.513	-17.611	-8.560	1.00	50.82
	ATOM	3869	O	ILE	C	689	13.616	-17.550	-9.097	1.00	51.28
	ATOM	3870	N	LEU	C	690	12.288	-17.162	-7.329	1.00	48.01
	ATOM	3871	CA	LEU	C	690	13.362	-16.570	-6.534	1.00	47.33
	ATOM	3872	CB	LEU	C	690	12.812	-16.058	-5.199	1.00	42.51
15	ATOM	3873	CG	LEU	C	690	13.835	-15.501	-4.206	1.00	40.67
	ATOM	3874	CD1	LEU	C	690	14.575	-14.324	-4.831	1.00	39.95
	ATOM	3875	CD2	LEU	C	690	13.128	-15.078	-2.926	1.00	38.77
	ATOM	3876	C	LEU	C	690	14.445	-17.615	-6.282	1.00	48.87
	ATOM	3877	O	LEU	C	690	15.643	-17.340	-6.393	1.00	46.71
20	ATOM	3878	N	HIS	C	691	14.001	-18.818	-5.939	1.00	51.36
	ATOM	3879	CA	HIS	C	691	14.886	-19.946	-5.675	1.00	53.35
	ATOM	3880	CB	HIS	C	691	14.042	-21.203	-5.460	1.00	58.64
	ATOM	3881	CG	HIS	C	691	14.655	-22.195	-4.526	1.00	62.94
	ATOM	3882	CD2	HIS	C	691	15.503	-23.227	-4.751	1.00	64.95
25	ATOM	3883	ND1	HIS	C	691	14.392	-22.202	-3.173	1.00	65.49
	ATOM	3884	CE1	HIS	C	691	15.053	-23.195	-2.605	1.00	68.18
	ATOM	3885	NE2	HIS	C	691	15.733	-23.833	-3.540	1.00	68.77
	ATOM	3886	C	HIS	C	691	15.824	-20.162	-6.861	1.00	52.19
	ATOM	3887	O	HIS	C	691	17.048	-20.153	-6.717	1.00	47.53
30	ATOM	3888	N	ARG	C	692	15.222	-20.350	-8.032	1.00	52.37
	ATOM	3889	CA	ARG	C	692	15.949	-20.586	-9.271	1.00	52.90
	ATOM	3890	CB	ARG	C	692	14.955	-20.832	-10.410	1.00	54.04
	ATOM	3891	CG	ARG	C	692	15.575	-20.826	-11.797	1.00	57.52
	ATOM	3892	CD	ARG	C	692	14.528	-21.048	-12.874	1.00	58.25
35	ATOM	3893	NE	ARG	C	692	14.375	-19.878	-13.732	1.00	61.43
	ATOM	3894	CZ	ARG	C	692	13.218	-19.260	-13.951	1.00	64.32
	ATOM	3895	NH1	ARG	C	692	12.108	-19.706	-13.378	1.00	63.22
	ATOM	3896	NH2	ARG	C	692	13.171	-18.197	-14.746	1.00	65.93
	ATOM	3897	C	ARG	C	692	16.873	-19.434	-9.639	1.00	53.09
40	ATOM	3898	O	ARG	C	692	18.047	-19.644	-9.956	1.00	53.06
	ATOM	3899	N	LEU	C	693	16.338	-18.217	-9.607	1.00	50.73
	ATOM	3900	CA	LEU	C	693	17.125	-17.039	-9.945	1.00	49.53
	ATOM	3901	CB	LEU	C	693	16.249	-15.784	-9.881	1.00	49.56
	ATOM	3902	CG	LEU	C	693	15.781	-15.245	-11.239	1.00	49.78
45	ATOM	3903	CD1	LEU	C	693	15.219	-16.389	-12.079	1.00	50.30
	ATOM	3904	CD2	LEU	C	693	14.728	-14.170	-11.037	1.00	48.79
	ATOM	3905	C	LEU	C	693	18.318	-16.904	-9.006	1.00	48.38
	ATOM	3906	O	LEU	C	693	19.382	-16.426	-9.402	1.00	46.35
	ATOM	3907	N	LEU	C	694	18.135	-17.329	-7.761	1.00	46.74
50	ATOM	3908	CA	LEU	C	694	19.204	-17.272	-6.775	1.00	49.41
	ATOM	3909	CB	LEU	C	694	18.634	-17.415	-5.362	1.00	45.20
	ATOM	3910	CG	LEU	C	694	18.222	-16.128	-4.643	1.00	40.19
	ATOM	3911	CD1	LEU	C	694	17.456	-16.474	-3.371	1.00	41.65
	ATOM	3912	CD2	LEU	C	694	19.453	-15.307	-4.317	1.00	35.91
55	ATOM	3913	C	LEU	C	694	20.172	-18.417	-7.058	1.00	54.15
	ATOM	3914	O	LEU	C	694	21.370	-18.320	-6.776	1.00	53.55
	ATOM	3915	N	GLN	C	695	19.634	-19.498	-7.619	1.00	57.44
	ATOM	3916	CA	GLN	C	695	20.416	-20.685	-7.959	1.00	62.46
	ATOM	3917	CB	GLN	C	695	19.477	-21.853	-8.304	1.00	61.95
60	ATOM	3918	CG	GLN	C	695	19.548	-23.010	-7.311	1.00	61.49
	ATOM	3919	CD	GLN	C	695	18.454	-24.053	-7.490	1.00	62.78

5	ATOM	3920	OE1	GLN	C	695	18.262	-24.928	-6.653	1.00	63.33
	ATOM	3921	NE2	GLN	C	695	17.720	-23.969	-8.608	1.00	60.37
	ATOM	3922	C	GLN	C	695	21.330	-20.414	-9.149	1.00	65.13
	ATOM	3923	O	GLN	C	695	22.517	-20.740	-9.116	1.00	65.87
	ATOM	3924	N	ASP	C	696	20.761	-19.824	-10.197	1.00	67.67
10	ATOM	3925	CA	ASP	C	696	21.492	-19.500	-11.420	1.00	70.66
	ATOM	3926	CB	ASP	C	696	20.801	-18.348	-12.151	1.00	71.06
	ATOM	3927	CG	ASP	C	696	20.127	-18.792	-13.430	1.00	71.70
	ATOM	3928	OD1	ASP	C	696	20.637	-18.455	-14.521	1.00	72.47
	ATOM	3929	OD2	ASP	C	696	19.086	-19.478	-13.342	1.00	71.41
15	ATOM	3930	C	ASP	C	696	22.951	-19.132	-11.169	1.00	72.41
	ATOM	3931	O	ASP	C	696	23.245	-18.115	-10.541	1.00	72.56
	ATOM	3932	N	SER	C	697	23.859	-19.967	-11.668	1.00	74.67
	ATOM	3933	CA	SER	C	697	25.291	-19.741	-11.507	1.00	76.45
	ATOM	3934	CB	SER	C	697	26.019	-21.076	-11.377	1.00	76.00
20	ATOM	3935	C	SER	C	697	25.841	-18.960	-12.696	1.00	78.44
	ATOM	3936	O	SER	C	697	26.286	-17.809	-12.489	1.00	79.20
	ATOM	3937	OXT	SER	C	697	25.818	-19.510	-13.820	1.00	80.07
	ATOM	3938	CB	LYS	D	686	-14.070	13.661	16.843	1.00	50.28
	ATOM	3939	C	LYS	D	686	-13.682	14.418	19.199	1.00	51.59
25	ATOM	3940	O	LYS	D	686	-12.629	14.738	19.759	1.00	50.42
	ATOM	3941	N	LYS	D	686	-12.910	15.796	17.283	1.00	50.43
	ATOM	3942	CA	LYS	D	686	-13.976	14.872	17.769	1.00	50.62
	ATOM	3943	N	HIS	D	687	-14.617	13.676	19.787	1.00	49.91
	ATOM	3944	CA	HIS	D	687	-14.447	13.176	21.144	1.00	51.28
30	ATOM	3945	CB	HIS	D	687	-15.806	12.984	21.828	1.00	54.12
	ATOM	3946	CG	HIS	D	687	-15.713	12.336	23.177	1.00	60.06
	ATOM	3947	CD2	HIS	D	687	-15.418	11.064	23.539	1.00	61.05
	ATOM	3948	ND1	HIS	D	687	-15.911	13.030	24.352	1.00	62.39
	ATOM	3949	CE1	HIS	D	687	-15.741	12.215	25.378	1.00	62.76
35	ATOM	3950	NE2	HIS	D	687	-15.441	11.016	24.912	1.00	63.46
	ATOM	3951	C	HIS	D	687	-13.691	11.849	21.163	1.00	49.55
	ATOM	3952	O	HIS	D	687	-14.099	10.878	20.524	1.00	50.84
	ATOM	3953	N	LYS	D	688	-12.593	11.816	21.909	1.00	44.00
	ATOM	3954	CA	LYS	D	688	-11.784	10.611	22.038	1.00	40.31
40	ATOM	3955	CB	LYS	D	688	-10.446	10.773	21.299	1.00	41.42
	ATOM	3956	CG	LYS	D	688	-10.513	10.595	19.780	1.00	42.76
	ATOM	3957	CD	LYS	D	688	-9.123	10.716	19.152	1.00	38.66
	ATOM	3958	CE	LYS	D	688	-9.162	10.529	17.640	1.00	38.28
	ATOM	3959	NZ	LYS	D	688	-7.894	10.970	16.986	1.00	31.58
45	ATOM	3960	C	LYS	D	688	-11.506	10.378	23.517	1.00	36.70
	ATOM	3961	O	LYS	D	688	-11.271	11.326	24.266	1.00	33.38
	ATOM	3962	N	ILE	D	689	-11.549	9.122	23.942	1.00	33.06
	ATOM	3963	CA	ILE	D	689	-11.255	8.806	25.328	1.00	28.70
	ATOM	3964	CB	ILE	D	689	-11.438	7.301	25.607	1.00	30.88
50	ATOM	3965	CG2	ILE	D	689	-10.725	6.912	26.899	1.00	31.45
	ATOM	3966	CG1	ILE	D	689	-12.927	6.971	25.721	1.00	32.57
	ATOM	3967	CD1	ILE	D	689	-13.308	5.679	25.031	1.00	29.79
	ATOM	3968	C	ILE	D	689	-9.790	9.193	25.541	1.00	27.64
	ATOM	3969	O	ILE	D	689	-9.405	9.649	26.611	1.00	25.54
55	ATOM	3970	N	LEU	D	690	-8.985	9.021	24.496	1.00	24.25
	ATOM	3971	CA	LEU	D	690	-7.563	9.348	24.549	1.00	26.63
	ATOM	3972	CB	LEU	D	690	-6.903	9.021	23.200	1.00	22.83
	ATOM	3973	CG	LEU	D	690	-5.433	9.387	22.992	1.00	25.47
	ATOM	3974	CD1	LEU	D	690	-4.595	8.772	24.108	1.00	24.03
60	ATOM	3975	CD2	LEU	D	690	-4.956	8.898	21.616	1.00	20.87
	ATOM	3976	C	LEU	D	690	-7.344	10.823	24.902	1.00	26.64



5	ATOM	3977	O	LEU	D	690	-6.408	11.165	25.625	1.00	28.34
	ATOM	3978	N	HIS	D	691	-8.206	11.694	24.383	1.00	27.77
	ATOM	3979	CA	HIS	D	691	-8.107	13.125	24.665	1.00	29.16
	ATOM	3980	CB	HIS	D	691	-9.156	13.907	23.861	1.00	30.89
	ATOM	3981	CG	HIS	D	691	-8.903	13.935	22.386	1.00	37.09
10	ATOM	3982	CD2	HIS	D	691	-7.750	14.000	21.679	1.00	41.39
	ATOM	3983	ND1	HIS	D	691	-9.920	13.906	21.458	1.00	41.65
	ATOM	3984	CE1	HIS	D	691	-9.407	13.953	20.242	1.00	44.64
	ATOM	3985	NE2	HIS	D	691	-8.091	14.010	20.347	1.00	41.94
	ATOM	3986	C	HIS	D	691	-8.338	13.373	26.159	1.00	26.65
15	ATOM	3987	O	HIS	D	691	-7.602	14.120	26.802	1.00	24.50
	ATOM	3988	N	ARG	D	692	-9.371	12.742	26.703	1.00	25.70
	ATOM	3989	CA	ARG	D	692	-9.691	12.912	28.114	1.00	29.11
	ATOM	3990	CB	ARG	D	692	-10.959	12.134	28.472	1.00	30.84
	ATOM	3991	CG	ARG	D	692	-11.255	12.129	29.963	1.00	41.63
20	ATOM	3992	CD	ARG	D	692	-12.502	11.327	30.290	1.00	48.83
	ATOM	3993	NE	ARG	D	692	-13.618	12.198	30.647	1.00	54.50
	ATOM	3994	CZ	ARG	D	692	-14.498	12.677	29.774	1.00	59.37
	ATOM	3995	NH1	ARG	D	692	-14.392	12.371	28.486	1.00	60.97
	ATOM	3996	NH2	ARG	D	692	-15.483	13.464	30.188	1.00	59.07
25	ATOM	3997	C	ARG	D	692	-8.548	12.451	29.011	1.00	28.30
	ATOM	3998	O	ARG	D	692	-8.139	13.167	29.929	1.00	26.50
	ATOM	3999	N	LEU	D	693	-8.030	11.259	28.737	1.00	24.87
	ATOM	4000	CA	LEU	D	693	-6.943	10.705	29.536	1.00	27.17
	ATOM	4001	CB	LEU	D	693	-6.674	9.254	29.116	1.00	28.45
30	ATOM	4002	CG	LEU	D	693	-7.844	8.300	29.391	1.00	30.40
	ATOM	4003	CD1	LEU	D	693	-7.575	6.932	28.778	1.00	34.79
	ATOM	4004	CD2	LEU	D	693	-8.043	8.171	30.894	1.00	32.02
	ATOM	4005	C	LEU	D	693	-5.670	11.539	29.440	1.00	25.96
	ATOM	4006	O	LEU	D	693	-4.948	11.700	30.428	1.00	27.01
35	ATOM	4007	N	LEU	D	694	-5.395	12.080	28.257	1.00	25.33
	ATOM	4008	CA	LEU	D	694	-4.207	12.906	28.062	1.00	27.22
	ATOM	4009	CB	LEU	D	694	-3.948	13.126	26.572	1.00	24.61
	ATOM	4010	CG	LEU	D	694	-3.118	12.080	25.825	1.00	22.20
	ATOM	4011	CD1	LEU	D	694	-3.230	12.332	24.324	1.00	21.13
40	ATOM	4012	CD2	LEU	D	694	-1.666	12.148	26.275	1.00	21.34
	ATOM	4013	C	LEU	D	694	-4.336	14.270	28.742	1.00	32.40
	ATOM	4014	O	LEU	D	694	-3.339	14.889	29.102	1.00	31.55
	ATOM	4015	N	GLN	D	695	-5.570	14.733	28.915	1.00	36.93
	ATOM	4016	CA	GLN	D	695	-5.820	16.032	29.528	1.00	43.18
45	ATOM	4017	CB	GLN	D	695	-7.022	16.694	28.862	1.00	40.48
	ATOM	4018	CG	GLN	D	695	-6.772	17.071	27.422	1.00	37.99
	ATOM	4019	CD	GLN	D	695	-7.943	17.764	26.795	1.00	35.86
	ATOM	4020	OE1	GLN	D	695	-7.863	18.895	26.342	1.00	38.84
	ATOM	4021	NE2	GLN	D	695	-9.082	17.060	26.757	1.00	31.62
50	ATOM	4022	C	GLN	D	695	-6.049	16.009	31.034	1.00	48.74
	ATOM	4023	O	GLN	D	695	-6.119	17.065	31.660	1.00	51.25
	ATOM	4024	N	ASP	D	696	-6.175	14.818	31.611	1.00	54.01
	ATOM	4025	CA	ASP	D	696	-6.398	14.702	33.047	1.00	62.23
	ATOM	4026	CB	ASP	D	696	-6.217	13.238	33.485	1.00	63.97
55	ATOM	4027	CG	ASP	D	696	-7.527	12.467	33.475	1.00	67.72
	ATOM	4028	OD1	ASP	D	696	-8.528	12.996	32.941	1.00	68.11
	ATOM	4029	OD2	ASP	D	696	-7.552	11.333	34.003	1.00	68.95
	ATOM	4030	C	ASP	D	696	-5.456	15.622	33.840	1.00	65.60
	ATOM	4031	O	ASP	D	696	-4.312	15.189	34.134	1.00	68.33
60	ATOM	4032	OXT	ASP	D	696	-5.874	16.755	34.140	1.00	69.20
	HETATM	4033	O	HOH		1	16.153	-0.605	-4.425	1.00	17.11

5	HETATM	4034	O	HOH	2	16.570	-5.304	-16.560	1.00	21.44
	HETATM	4035	O	HOH	3	18.526	0.742	-4.495	1.00	23.43
	HETATM	4036	O	HOH	4	13.647	-2.187	8.588	1.00	25.82
	HETATM	4037	O	HOH	5	9.778	-5.825	2.509	1.00	20.58
	HETATM	4038	O	HOH	6	17.072	-3.605	-8.015	1.00	18.38
10	HETATM	4039	O	HOH	7	24.920	-1.689	-2.780	1.00	25.74
	HETATM	4040	O	HOH	8	7.321	-5.649	5.061	1.00	24.11
	HETATM	4041	O	HOH	9	25.976	-3.535	15.158	1.00	26.78
	HETATM	4042	O	HOH	10	15.088	-7.006	-15.192	1.00	19.64
	HETATM	4043	O	HOH	11	14.070	0.925	-5.953	1.00	20.55
15	HETATM	4044	O	HOH	12	18.008	3.407	-6.654	1.00	32.30
	HETATM	4045	O	HOH	13	31.949	-8.393	13.487	1.00	30.64
	HETATM	4046	O	HOH	14	19.625	-2.804	-4.279	1.00	24.45
	HETATM	4047	O	HOH	15	11.741	1.079	-21.140	1.00	25.87
	HETATM	4048	O	HOH	16	25.067	13.951	14.153	1.00	31.07
20	HETATM	4049	O	HOH	17	15.501	1.323	-10.393	1.00	21.01
	HETATM	4050	O	HOH	18	13.880	3.349	-11.482	1.00	24.28
	HETATM	4051	O	HOH	19	17.591	0.979	-8.828	1.00	35.26
	HETATM	4052	O	HOH	20	23.682	-2.041	-0.314	1.00	37.90
	HETATM	4053	O	HOH	21	15.754	9.496	11.841	1.00	39.44
25	HETATM	4054	O	HOH	22	-4.943	7.574	-3.066	1.00	37.67
	HETATM	4055	O	HOH	23	6.877	0.354	-15.982	1.00	36.92
	HETATM	4056	O	HOH	24	15.806	-4.002	8.671	1.00	30.38
	HETATM	4057	O	HOH	25	17.185	-3.158	-5.321	1.00	28.89
	HETATM	4058	O	HOH	26	17.572	9.249	17.009	1.00	30.15
30	HETATM	4059	O	HOH	27	24.096	-2.929	11.604	1.00	31.37
	HETATM	4060	O	HOH	28	22.324	-5.871	-11.980	1.00	32.74
	HETATM	4061	O	HOH	29	27.547	-12.361	-0.801	1.00	36.61
	HETATM	4062	O	HOH	30	11.173	13.442	-2.719	1.00	35.41
	HETATM	4063	O	HOH	31	15.438	-9.527	5.483	1.00	29.88
35	HETATM	4064	O	HOH	32	9.946	-6.564	5.983	1.00	35.05
	HETATM	4065	O	HOH	33	7.599	11.680	-15.261	1.00	38.68
	HETATM	4066	O	HOH	34	20.112	10.503	-5.109	1.00	42.66
	HETATM	4067	O	HOH	35	15.972	10.343	14.897	1.00	41.73
	HETATM	4068	O	HOH	36	22.401	-5.914	-9.527	1.00	28.08
40	HETATM	4069	O	HOH	37	16.128	-0.899	-8.109	1.00	33.13
	HETATM	4070	O	HOH	38	3.581	15.655	-3.706	1.00	41.37
	HETATM	4071	O	HOH	39	31.900	13.545	21.339	1.00	37.79
	HETATM	4072	O	HOH	40	20.058	-7.530	14.119	1.00	47.51
	HETATM	4073	O	HOH	41	34.634	6.668	15.632	1.00	29.24
45	HETATM	4074	O	HOH	42	17.968	10.511	-9.085	1.00	44.60
	HETATM	4075	O	HOH	43	23.258	-17.325	-4.088	1.00	44.10
	HETATM	4076	O	HOH	44	4.034	-1.472	27.521	1.00	15.22
	HETATM	4077	O	HOH	45	-5.943	-0.018	36.088	1.00	21.11
	HETATM	4078	O	HOH	46	6.084	-1.509	29.478	1.00	19.51
50	HETATM	4079	O	HOH	47	9.762	1.061	15.621	1.00	27.74
	HETATM	4080	O	HOH	48	1.804	0.717	17.260	1.00	20.97
	HETATM	4081	O	HOH	49	0.929	0.421	30.281	1.00	19.64
	HETATM	4082	O	HOH	50	9.627	4.271	31.231	1.00	19.02
	HETATM	4083	O	HOH	51	2.121	-0.261	13.654	1.00	26.09
55	HETATM	4084	O	HOH	52	20.060	10.275	17.711	1.00	25.49
	HETATM	4085	O	HOH	53	-6.786	0.736	33.483	1.00	22.34
	HETATM	4086	O	HOH	54	2.751	-4.136	27.760	1.00	19.93
	HETATM	4087	O	HOH	55	5.994	-4.079	31.292	1.00	32.27
	HETATM	4088	O	HOH	56	19.416	16.921	21.645	1.00	25.54
60	HETATM	4089	O	HOH	57	4.833	2.325	29.006	1.00	19.00
	HETATM	4090	O	HOH	58	-7.638	-8.931	37.809	1.00	24.79

5	HETATM	4091	O	HOH	59	28.442	-4.673	21.875	1.00	24.32
	HETATM	4092	O	HOH	60	1.094	-4.893	32.100	1.00	24.27
	HETATM	4093	O	HOH	61	0.905	-7.306	32.783	1.00	21.33
	HETATM	4094	O	HOH	62	3.396	-2.971	32.306	1.00	26.13
	HETATM	4095	O	HOH	63	10.363	4.576	28.391	1.00	33.43
10	HETATM	4096	O	HOH	64	19.551	-6.473	16.597	1.00	35.38
	HETATM	4097	O	HOH	65	-2.888	-19.627	15.665	1.00	27.99
	HETATM	4098	O	HOH	66	-7.275	-9.745	31.077	1.00	27.00
	HETATM	4099	O	HOH	67	10.189	3.580	16.510	1.00	24.19
	HETATM	4100	O	HOH	68	2.741	0.716	28.382	1.00	16.48
15	HETATM	4101	O	HOH	69	23.522	-4.323	13.943	1.00	27.48
	HETATM	4102	O	HOH	70	17.133	8.133	19.686	1.00	32.24
	HETATM	4103	O	HOH	71	-0.295	4.535	35.884	1.00	33.42
	HETATM	4104	O	HOH	72	9.519	10.828	34.842	1.00	29.38
	HETATM	4105	O	HOH	73	6.291	14.878	29.070	1.00	28.21
20	HETATM	4106	O	HOH	74	-1.721	6.480	13.381	1.00	49.91
	HETATM	4107	O	HOH	75	10.091	-15.427	26.194	1.00	24.17
	HETATM	4108	O	HOH	76	5.029	7.461	17.718	1.00	18.91
	HETATM	4109	O	HOH	77	3.758	2.086	14.306	1.00	28.28
	HETATM	4110	O	HOH	78	-1.390	-18.739	33.183	1.00	41.11
25	HETATM	4111	O	HOH	79	12.703	-8.687	32.119	1.00	36.21
	HETATM	4112	O	HOH	80	22.270	-6.451	14.844	1.00	33.21
	HETATM	4113	O	HOH	81	1.458	4.605	34.026	1.00	23.59
	HETATM	4114	O	HOH	82	1.759	-2.158	30.374	1.00	28.78
	HETATM	4115	O	HOH	83	6.153	-21.372	23.188	1.00	31.14
30	HETATM	4116	O	HOH	84	36.525	0.463	20.792	1.00	45.26
	HETATM	4117	O	HOH	85	13.832	9.696	13.792	1.00	33.12
	HETATM	4118	O	HOH	86	31.166	6.635	24.924	1.00	35.19
	HETATM	4119	O	HOH	87	8.844	-10.389	34.180	1.00	48.80
	HETATM	4120	O	HOH	88	9.581	-6.956	34.136	1.00	42.95
35	HETATM	4121	O	HOH	89	-1.563	15.887	27.596	1.00	39.35
	HETATM	4122	O	HOH	90	-5.286	10.345	32.757	1.00	35.20
	HETATM	4123	O	HOH	91	15.035	0.607	13.339	1.00	29.53
	HETATM	4124	O	HOH	92	-10.984	-1.500	30.272	1.00	29.84
	HETATM	4125	O	HOH	93	-7.239	-0.271	-1.207	1.00	48.98
40	HETATM	4126	O	HOH	94	18.022	-4.902	34.286	1.00	35.28
	HETATM	4127	O	HOH	95	29.347	-6.319	19.920	1.00	37.20
	HETATM	4128	O	HOH	96	-14.309	-19.369	20.945	1.00	30.23
	HETATM	4129	O	HOH	97	31.496	4.614	18.716	1.00	38.79
	HETATM	4130	O	HOH	98	26.567	9.759	25.629	1.00	29.72
45	HETATM	4131	O	HOH	99	2.848	14.531	1.134	1.00	38.08
	HETATM	4132	O	HOH	100	-9.373	5.699	-7.953	1.00	53.23
	HETATM	4133	O	HOH	101	-10.137	-0.553	-6.742	1.00	47.72
	HETATM	4134	O	HOH	102	10.558	-10.363	15.403	1.00	40.97
	HETATM	4135	O	HOH	103	21.079	17.166	18.929	1.00	32.40
50	HETATM	4136	O	HOH	104	25.810	-5.921	22.506	1.00	37.69
	HETATM	4137	O	HOH	105	22.493	-1.311	34.465	1.00	49.94
	HETATM	4138	O	HOH	106	19.317	10.977	38.703	1.00	40.60
	HETATM	4139	O	HOH	107	4.479	13.951	3.045	1.00	45.33
	HETATM	4140	O	HOH	108	20.418	19.353	34.044	1.00	42.18
55	HETATM	4141	O	HOH	109	-3.065	8.936	14.062	1.00	38.41
	HETATM	4142	O	HOH	110	26.856	-4.674	-10.940	1.00	55.67
	HETATM	4143	O	HOH	111	2.032	-6.387	5.614	1.00	42.23
	HETATM	4144	O	HOH	112	0.601	0.228	-17.268	1.00	40.57
	HETATM	4145	O	HOH	113	4.903	13.488	-14.050	1.00	47.72
60	HETATM	4146	O	HOH	114	3.986	16.140	-0.960	1.00	40.66
	HETATM	4147	O	HOH	115	12.968	-19.561	2.741	1.00	40.76

5	HETATM	4148	O	HOH	116	7.170	15.583	2.599	1.00	43.69
	HETATM	4149	O	HOH	117	-1.966	10.606	3.572	1.00	52.63
	HETATM	4150	O	HOH	118	29.030	10.644	6.707	1.00	42.54
	HETATM	4151	O	HOH	119	0.468	4.354	8.374	1.00	38.69
	HETATM	4152	O	HOH	120	29.086	17.119	19.272	1.00	45.51
10	HETATM	4153	O	HOH	121	24.614	17.609	20.174	1.00	53.55
	HETATM	4154	O	HOH	122	-15.318	0.362	26.686	1.00	36.77
	HETATM	4155	O	HOH	123	-3.857	-24.786	28.325	1.00	39.64
	HETATM	4156	O	HOH	124	21.728	22.178	31.983	1.00	43.73
	HETATM	4157	O	HOH	125	31.650	-7.370	21.642	1.00	40.53
15	HETATM	4158	O	HOH	126	25.421	10.436	21.161	1.00	32.31
	HETATM	4159	O	HOH	127	10.317	-9.457	12.998	1.00	37.77
	HETATM	4160	O	HOH	128	22.723	14.887	15.427	1.00	47.90
	HETATM	4161	O	HOH	129	6.702	9.556	37.596	1.00	47.81
	HETATM	4162	O	HOH	130	27.987	13.557	7.167	1.00	41.15
20	HETATM	4163	O	HOH	131	30.798	16.499	7.588	1.00	58.47
	HETATM	4164	O	HOH	132	10.071	-0.571	-20.393	1.00	38.79
	HETATM	4165	O	HOH	133	9.562	8.334	-21.392	1.00	36.80
	HETATM	4166	O	HOH	134	6.712	6.058	8.822	1.00	37.43
	HETATM	4167	O	HOH	135	5.927	8.454	10.594	1.00	42.34
25	HETATM	4168	O	HOH	136	4.472	6.306	10.973	1.00	37.35
	HETATM	4169	O	HOH	137	6.792	7.721	7.051	1.00	47.23
	HETATM	4170	O	HOH	138	24.513	11.582	33.724	1.00	45.55
	HETATM	4171	O	HOH	139	-2.528	-20.361	12.354	1.00	52.13
	HETATM	4172	O	HOH	140	-7.864	7.706	19.248	1.00	47.82
30	HETATM	4173	O	HOH	141	11.577	-16.962	24.398	1.00	39.43
	HETATM	4174	O	HOH	142	18.087	12.263	-5.507	1.00	33.36
	HETATM	4175	O	HOH	143	-6.816	-14.190	10.674	1.00	51.32
	HETATM	4176	O	HOH	144	-7.377	-16.701	33.528	1.00	57.11
	HETATM	4177	O	HOH	145	-5.379	-20.107	32.689	1.00	43.01
35	HETATM	4178	O	HOH	146	8.766	-7.947	-16.274	1.00	49.96
	HETATM	4179	O	HOH	147	10.946	-7.937	-18.142	1.00	55.67
	END									

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## Appendix 3

Atomic Coordinates for Human ER $\alpha$  Complexed With OHT

10	CRYST1	58.242	58.242	277.467	90.00	90.00	120.00	P	65	2	2	12
	ORIGX1	1.000000	0.000000	0.000000	0.000000	0.000000						
	ORIGX2	0.000000	1.000000	0.000000	0.000000	0.000000						
	ORIGX3	0.000000	0.000000	1.000000	0.000000	0.000000						
	SCALE1	0.017170	0.009913	0.000000	0.000000	0.000000						
15	SCALE2	0.000000	0.019826	0.000000	0.000000	0.000000						
	SCALE3	0.000000	0.000000	0.003604	0.000000	0.000000						
	ATOM	1	CB	LEU	306	6.638	11.502	3.989	1.00	61.20		
	ATOM	2	C	LEU	306	7.381	10.684	6.231	1.00	61.47		
20	ATOM	3	O	LEU	306	6.407	11.020	6.905	1.00	62.09		
	ATOM	4	N	LEU	306	6.369	9.128	4.588	1.00	62.32		
	ATOM	5	CA	LEU	306	7.232	10.330	4.754	1.00	61.30		
	ATOM	6	N	ALA	307	8.609	10.605	6.730	1.00	60.52		
	ATOM	7	CA	ALA	307	8.891	10.912	8.125	1.00	58.77		
25	ATOM	8	CB	ALA	307	10.318	10.501	8.465	1.00	59.70		
	ATOM	9	C	ALA	307	8.692	12.393	8.429	1.00	57.51		
	ATOM	10	O	ALA	307	8.451	12.770	9.574	1.00	57.64		
	ATOM	11	N	LEU	308	8.789	13.228	7.400	1.00	55.82		
	ATOM	12	CA	LEU	308	8.638	14.668	7.573	1.00	56.62		
30	ATOM	13	CB	LEU	308	9.298	15.402	6.406	1.00	57.48		
	ATOM	14	CG	LEU	308	10.637	14.822	5.948	1.00	59.17		
	ATOM	15	CD1	LEU	308	10.474	14.189	4.569	1.00	60.38		
	ATOM	16	CD2	LEU	308	11.694	15.920	5.933	1.00	58.46		
	ATOM	17	C	LEU	308	7.190	15.130	7.710	1.00	56.51		
35	ATOM	18	O	LEU	308	6.935	16.307	7.961	1.00	55.58		
	ATOM	19	N	SER	309	6.246	14.208	7.546	1.00	57.04		
	ATOM	20	CA	SER	309	4.828	14.544	7.657	1.00	56.46		
	ATOM	21	CB	SER	309	4.034	13.896	6.514	1.00	56.79		
	ATOM	22	OG	SER	309	4.071	12.479	6.588	1.00	57.23		
40	ATOM	23	C	SER	309	4.261	14.095	9.003	1.00	56.13		
	ATOM	24	O	SER	309	3.166	14.507	9.398	1.00	55.17		
	ATOM	25	N	LEU	310	5.016	13.257	9.706	1.00	54.31		
	ATOM	26	CA	LEU	310	4.591	12.749	11.004	1.00	53.55		
	ATOM	27	CB	LEU	310	5.651	11.811	11.582	1.00	54.40		
45	ATOM	28	CG	LEU	310	5.586	10.333	11.189	1.00	56.49		
	ATOM	29	CD1	LEU	310	5.530	10.200	9.676	1.00	57.06		
	ATOM	30	CD2	LEU	310	6.809	9.610	11.739	1.00	57.28		
	ATOM	31	C	LEU	310	4.330	13.865	12.003	1.00	53.18		
	ATOM	32	O	LEU	310	4.993	14.905	11.984	1.00	53.17		
50	ATOM	33	N	THR	311	3.352	13.641	12.874	1.00	51.71		
	ATOM	34	CA	THR	311	3.017	14.604	13.912	1.00	49.93		
	ATOM	35	CB	THR	311	1.527	14.554	14.275	1.00	48.96		
	ATOM	36	OG1	THR	311	1.242	13.311	14.930	1.00	47.20		
	ATOM	37	CG2	THR	311	0.666	14.688	13.027	1.00	50.99		
55	ATOM	38	C	THR	311	3.815	14.201	15.145	1.00	48.84		
	ATOM	39	O	THR	311	4.371	13.103	15.197	1.00	46.66		
	ATOM	40	N	ALA	312	3.857	15.078	16.141	1.00	48.76		
	ATOM	41	CA	ALA	312	4.590	14.798	17.369	1.00	47.75		
	ATOM	42	CB	ALA	312	4.359	15.910	18.378	1.00	47.06		
60	ATOM	43	C	ALA	312	4.171	13.460	17.964	1.00	47.41		

5	ATOM	44	O	ALA	312	5.009	12.609	18.262	1.00	45.52
	ATOM	45	N	ASP	313	2.868	13.275	18.143	1.00	47.58
	ATOM	46	CA	ASP	313	2.367	12.032	18.714	1.00	47.63
	ATOM	47	CB	ASP	313	0.848	12.100	18.879	1.00	51.96
	ATOM	48	CG	ASP	313	0.430	12.872	20.118	1.00	56.21
10	ATOM	49	OD1	ASP	313	1.314	13.234	20.929	1.00	56.38
	ATOM	50	OD2	ASP	313	-0.785	13.117	20.282	1.00	59.15
	ATOM	51	C	ASP	313	2.745	10.846	17.835	1.00	43.93
	ATOM	52	O	ASP	313	2.959	9.741	18.330	1.00	44.77
	ATOM	53	N	GLN	314	2.826	11.081	16.531	1.00	44.52
15	ATOM	54	CA	GLN	314	3.182	10.028	15.588	1.00	44.73
	ATOM	55	CB	GLN	314	2.849	10.464	14.156	1.00	45.05
	ATOM	56	CG	GLN	314	1.534	9.886	13.626	1.00	48.47
	ATOM	57	CD	GLN	314	0.982	10.646	12.428	1.00	50.37
	ATOM	58	OE1	GLN	314	1.649	11.515	11.856	1.00	49.38
20	ATOM	59	NE2	GLN	314	-0.248	10.318	12.043	1.00	51.74
	ATOM	60	C	GLN	314	4.673	9.722	15.707	1.00	43.26
	ATOM	61	O	GLN	314	5.100	8.580	15.555	1.00	43.93
	ATOM	62	N	MET	315	5.459	10.757	15.980	1.00	42.29
	ATOM	63	CA	MET	315	6.901	10.606	16.130	1.00	41.26
25	ATOM	64	CB	MET	315	7.565	11.985	16.224	1.00	42.43
	ATOM	65	CG	MET	315	9.082	11.939	16.356	1.00	42.34
	ATOM	66	SD	MET	315	9.906	11.190	14.925	1.00	46.22
	ATOM	67	CE	MET	315	9.547	12.408	13.680	1.00	37.32
	ATOM	68	C	MET	315	7.218	9.791	17.379	1.00	38.89
30	ATOM	69	O	MET	315	8.002	8.841	17.335	1.00	40.02
	ATOM	70	N	VAL	316	6.599	10.165	18.491	1.00	37.65
	ATOM	71	CA	VAL	316	6.819	9.476	19.756	1.00	39.56
	ATOM	72	CB	VAL	316	6.023	10.136	20.897	1.00	39.22
	ATOM	73	CG1	VAL	316	6.245	9.373	22.192	1.00	44.43
35	ATOM	74	CG2	VAL	316	6.446	11.583	21.059	1.00	41.04
	ATOM	75	C	VAL	316	6.404	8.012	19.664	1.00	40.04
	ATOM	76	O	VAL	316	7.141	7.117	20.077	1.00	37.86
	ATOM	77	N	SER	317	5.215	7.767	19.127	1.00	41.90
	ATOM	78	CA	SER	317	4.733	6.400	18.997	1.00	41.68
40	ATOM	79	CB	SER	317	3.311	6.402	18.415	1.00	43.85
	ATOM	80	OG	SER	317	3.225	5.631	17.230	1.00	49.38
	ATOM	81	C	SER	317	5.696	5.601	18.114	1.00	39.72
	ATOM	82	O	SER	317	6.011	4.446	18.407	1.00	40.21
	ATOM	83	N	ALA	318	6.182	6.220	17.043	1.00	38.35
45	ATOM	84	CA	ALA	318	7.114	5.540	16.153	1.00	36.96
	ATOM	85	CB	ALA	318	7.485	6.448	14.986	1.00	37.92
	ATOM	86	C	ALA	318	8.375	5.137	16.920	1.00	38.31
	ATOM	87	O	ALA	318	8.820	3.992	16.844	1.00	33.94
	ATOM	88	N	LEU	319	8.938	6.089	17.664	1.00	36.92
50	ATOM	89	CA	LEU	319	10.161	5.854	18.438	1.00	38.56
	ATOM	90	CB	LEU	319	10.660	7.174	19.040	1.00	40.86
	ATOM	91	CG	LEU	319	11.136	8.264	18.071	1.00	41.25
	ATOM	92	CD1	LEU	319	11.714	9.440	18.857	1.00	44.30
	ATOM	93	CD2	LEU	319	12.182	7.693	17.140	1.00	42.61
55	ATOM	94	C	LEU	319	9.965	4.826	19.549	1.00	38.33
	ATOM	95	O	LEU	319	10.779	3.916	19.729	1.00	33.91
	ATOM	96	N	LEU	320	8.879	4.982	20.297	1.00	37.39
	ATOM	97	CA	LEU	320	8.567	4.067	21.387	1.00	41.55
	ATOM	98	CB	LEU	320	7.239	4.467	22.049	1.00	38.47
60	ATOM	99	CG	LEU	320	7.236	5.582	23.099	1.00	44.81
	ATOM	100	CD1	LEU	320	5.876	5.634	23.802	1.00	44.96

5	ATOM	101	CD2	LEU	320	8.334	5.332	24.112	1.00	43.36
	ATOM	102	C	LEU	320	8.466	2.642	20.843	1.00	41.11
	ATOM	103	O	LEU	320	8.971	1.697	21.443	1.00	41.87
	ATOM	104	N	ASP	321	7.812	2.504	19.696	1.00	43.94
	ATOM	105	CA	ASP	321	7.613	1.210	19.053	1.00	44.77
10	ATOM	106	CB	ASP	321	6.669	1.372	17.860	1.00	48.39
	ATOM	107	CG	ASP	321	5.206	1.318	18.255	1.00	52.39
	ATOM	108	OD1	ASP	321	4.901	1.422	19.464	1.00	53.56
	ATOM	109	OD2	ASP	321	4.357	1.172	17.346	1.00	55.81
	ATOM	110	C	ASP	321	8.911	0.565	18.568	1.00	44.37
15	ATOM	111	O	ASP	321	9.030	-0.661	18.533	1.00	44.67
	ATOM	112	N	ALA	322	9.878	1.395	18.193	1.00	40.75
	ATOM	113	CA	ALA	322	11.153	0.905	17.686	1.00	37.81
	ATOM	114	CB	ALA	322	11.772	1.954	16.776	1.00	38.07
	ATOM	115	C	ALA	322	12.148	0.513	18.769	1.00	35.52
20	ATOM	116	O	ALA	322	13.219	-0.020	18.473	1.00	36.11
	ATOM	117	N	GLU	323	11.799	0.768	20.022	1.00	35.61
	ATOM	118	CA	GLU	323	12.704	0.460	21.117	1.00	36.39
	ATOM	119	CB	GLU	323	12.042	0.768	22.459	1.00	35.09
	ATOM	120	CG	GLU	323	12.209	2.210	22.899	1.00	37.93
25	ATOM	121	CD	GLU	323	13.657	2.569	23.200	1.00	37.29
	ATOM	122	OE1	GLU	323	14.313	3.173	22.326	1.00	34.21
	ATOM	123	OE2	GLU	323	14.134	2.245	24.309	1.00	38.02
	ATOM	124	C	GLU	323	13.205	-0.978	21.110	1.00	38.01
	ATOM	125	O	GLU	323	12.425	-1.931	20.999	1.00	38.37
30	ATOM	126	N	PRO	324	14.527	-1.151	21.225	1.00	36.03
	ATOM	127	CD	PRO	324	15.522	-0.069	21.345	1.00	36.69
	ATOM	128	CA	PRO	324	15.158	-2.474	21.240	1.00	36.42
	ATOM	129	CB	PRO	324	16.633	-2.166	21.003	1.00	35.75
	ATOM	130	CG	PRO	324	16.811	-0.807	21.610	1.00	35.46
35	ATOM	131	C	PRO	324	14.940	-3.162	22.583	1.00	35.75
	ATOM	132	O	PRO	324	14.616	-2.517	23.580	1.00	34.97
	ATOM	133	N	PRO	325	15.134	-4.485	22.631	1.00	35.24
	ATOM	134	CD	PRO	325	15.530	-5.386	21.534	1.00	37.02
	ATOM	135	CA	PRO	325	14.942	-5.208	23.889	1.00	34.65
40	ATOM	136	CB	PRO	325	14.753	-6.652	23.439	1.00	35.83
	ATOM	137	CG	PRO	325	15.589	-6.743	22.200	1.00	34.88
	ATOM	138	C	PRO	325	16.132	-5.070	24.824	1.00	34.51
	ATOM	139	O	PRO	325	17.237	-4.723	24.399	1.00	29.92
	ATOM	140	N	ILE	326	15.899	-5.322	26.106	1.00	33.62
45	ATOM	141	CA	ILE	326	16.975	-5.265	27.075	1.00	35.02
	ATOM	142	CB	ILE	326	16.458	-4.891	28.473	1.00	38.11
	ATOM	143	CG2	ILE	326	17.557	-5.110	29.504	1.00	38.70
	ATOM	144	CG1	ILE	326	15.987	-3.431	28.466	1.00	40.48
	ATOM	145	CD1	ILE	326	16.035	-2.747	29.815	1.00	42.96
50	ATOM	146	C	ILE	326	17.567	-6.668	27.103	1.00	34.14
	ATOM	147	O	ILE	326	16.875	-7.634	27.427	1.00	34.88
	ATOM	148	N	LEU	327	18.840	-6.784	26.745	1.00	29.64
	ATOM	149	CA	LEU	327	19.493	-8.083	26.716	1.00	29.54
	ATOM	150	CB	LEU	327	20.528	-8.135	25.587	1.00	27.76
55	ATOM	151	CG	LEU	327	19.978	-7.800	24.196	1.00	29.02
	ATOM	152	CD1	LEU	327	21.068	-7.993	23.139	1.00	28.76
	ATOM	153	CD2	LEU	327	18.775	-8.688	23.891	1.00	31.26
	ATOM	154	C	LEU	327	20.156	-8.438	28.030	1.00	31.21
	ATOM	155	O	LEU	327	20.393	-7.578	28.891	1.00	30.12
60	ATOM	156	N	TYR	328	20.445	-9.725	28.181	1.00	30.99
	ATOM	157	CA	TYR	328	21.087	-10.229	29.381	1.00	30.95

5	ATOM	158	CB	TYR	328	20.409	-11.520	29.842	1.00	33.38
	ATOM	159	CG	TYR	328	19.194	-11.272	30.686	1.00	33.05
	ATOM	160	CD1	TYR	328	19.253	-11.398	32.071	1.00	31.92
	ATOM	161	CE1	TYR	328	18.152	-11.114	32.864	1.00	36.01
	ATOM	162	CD2	TYR	328	17.996	-10.862	30.110	1.00	36.05
10	ATOM	163	CE2	TYR	328	16.880	-10.574	30.899	1.00	37.27
	ATOM	164	CZ	TYR	328	16.973	-10.702	32.274	1.00	37.66
	ATOM	165	OH	TYR	328	15.896	-10.397	33.071	1.00	44.66
	ATOM	166	C	TYR	328	22.529	-10.520	29.067	1.00	33.66
	ATOM	167	O	TYR	328	22.884	-10.744	27.910	1.00	34.78
15	ATOM	168	N	SER	329	23.359	-10.496	30.103	1.00	33.97
	ATOM	169	CA	SER	329	24.767	-10.800	29.962	1.00	37.29
	ATOM	170	CB	SER	329	25.526	-10.342	31.204	1.00	36.51
	ATOM	171	OG	SER	329	26.787	-10.965	31.282	1.00	37.13
	ATOM	172	C	SER	329	24.835	-12.317	29.832	1.00	40.43
20	ATOM	173	O	SER	329	23.980	-13.028	30.363	1.00	40.11
	ATOM	174	N	GLU	330	25.845	-12.811	29.128	1.00	41.40
	ATOM	175	CA	GLU	330	25.992	-14.242	28.928	1.00	47.43
	ATOM	176	CB	GLU	330	26.423	-14.524	27.484	1.00	48.64
	ATOM	177	CG	GLU	330	25.278	-14.870	26.542	1.00	50.20
25	ATOM	178	CD	GLU	330	25.765	-15.405	25.198	1.00	53.25
	ATOM	179	OE1	GLU	330	25.909	-16.640	25.062	1.00	53.27
	ATOM	180	OE2	GLU	330	26.004	-14.590	24.280	1.00	51.80
	ATOM	181	C	GLU	330	26.999	-14.852	29.893	1.00	49.67
	ATOM	182	O	GLU	330	28.207	-14.741	29.696	1.00	50.11
30	ATOM	183	N	TYR	331	26.498	-15.493	30.942	1.00	53.62
	ATOM	184	CA	TYR	331	27.373	-16.130	31.921	1.00	58.16
	ATOM	185	CB	TYR	331	28.092	-15.078	32.774	1.00	59.55
	ATOM	186	CG	TYR	331	27.239	-14.460	33.860	1.00	63.08
	ATOM	187	CD1	TYR	331	26.656	-13.205	33.682	1.00	64.50
35	ATOM	188	CE1	TYR	331	25.864	-12.630	34.676	1.00	65.99
	ATOM	189	CD2	TYR	331	27.010	-15.128	35.065	1.00	63.52
	ATOM	190	CE2	TYR	331	26.219	-14.563	36.066	1.00	65.60
	ATOM	191	CZ	TYR	331	25.648	-13.314	35.864	1.00	67.20
	ATOM	192	OH	TYR	331	24.855	-12.753	36.839	1.00	67.40
40	ATOM	193	C	TYR	331	26.603	-17.080	32.823	1.00	59.05
	ATOM	194	O	TYR	331	25.393	-16.942	33.002	1.00	59.22
	ATOM	195	N	ASP	332	27.320	-18.045	33.387	1.00	61.62
	ATOM	196	CA	ASP	332	26.719	-19.026	34.281	1.00	64.20
	ATOM	197	CB	ASP	332	27.681	-20.194	34.500	1.00	65.99
45	ATOM	198	CG	ASP	332	26.961	-21.516	34.648	1.00	68.11
	ATOM	199	OD1	ASP	332	27.575	-22.564	34.351	1.00	69.54
	ATOM	200	OD2	ASP	332	25.781	-21.505	35.060	1.00	67.40
	ATOM	201	C	ASP	332	26.393	-18.371	35.619	1.00	63.33
	ATOM	202	O	ASP	332	27.292	-18.073	36.406	1.00	63.90
50	ATOM	203	N	PRO	333	25.096	-18.148	35.896	1.00	63.64
	ATOM	204	CD	PRO	333	23.945	-18.509	35.053	1.00	64.35
	ATOM	205	CA	PRO	333	24.677	-17.521	37.154	1.00	63.52
	ATOM	206	CB	PRO	333	23.165	-17.333	36.993	1.00	63.53
	ATOM	207	CG	PRO	333	22.866	-17.611	35.556	1.00	64.15
55	ATOM	208	C	PRO	333	25.010	-18.419	38.332	1.00	63.29
	ATOM	209	O	PRO	333	25.129	-17.964	39.468	1.00	63.28
	ATOM	210	N	THR	334	25.160	-19.704	38.037	1.00	64.26
	ATOM	211	CA	THR	334	25.475	-20.697	39.050	1.00	66.09
	ATOM	212	CB	THR	334	24.929	-22.080	38.645	1.00	66.90
60	ATOM	213	OG1	THR	334	25.571	-22.513	37.439	1.00	68.06
	ATOM	214	CG2	THR	334	23.423	-22.012	38.411	1.00	67.57



5	ATOM	215	C	THR	334	26.982	-20.804	39.269	1.00	65.67
	ATOM	216	O	THR	334	27.432	-21.323	40.289	1.00	64.77
	ATOM	217	N	ARG	335	27.759	-20.308	38.313	1.00	65.65
	ATOM	218	CA	ARG	335	29.214	-20.360	38.421	1.00	66.60
	ATOM	219	CB	ARG	335	29.835	-20.500	37.030	1.00	66.74
10	ATOM	220	C	ARG	335	29.757	-19.113	39.123	1.00	67.09
	ATOM	221	O	ARG	335	29.100	-18.071	39.148	1.00	67.31
	ATOM	222	N	PRO	336	30.968	-19.207	39.702	1.00	67.62
	ATOM	223	CD	PRO	336	31.820	-20.408	39.713	1.00	67.30
	ATOM	224	CA	PRO	336	31.601	-18.086	40.410	1.00	67.42
15	ATOM	225	CB	PRO	336	32.982	-18.621	40.783	1.00	66.43
	ATOM	226	CG	PRO	336	32.829	-20.097	40.779	1.00	67.52
	ATOM	227	C	PRO	336	31.701	-16.828	39.561	1.00	68.26
	ATOM	228	O	PRO	336	31.996	-16.895	38.371	1.00	69.04
	ATOM	229	N	PHE	337	31.460	-15.681	40.183	1.00	69.49
20	ATOM	230	CA	PHE	337	31.529	-14.408	39.480	1.00	71.39
	ATOM	231	CB	PHE	337	30.818	-13.323	40.294	1.00	72.31
	ATOM	232	CG	PHE	337	31.219	-11.924	39.921	1.00	73.21
	ATOM	233	CD1	PHE	337	30.632	-11.287	38.833	1.00	72.82
	ATOM	234	CD2	PHE	337	32.191	-11.245	40.653	1.00	73.43
25	ATOM	235	CE1	PHE	337	31.006	-9.993	38.479	1.00	73.28
	ATOM	236	CE2	PHE	337	32.573	-9.950	40.306	1.00	73.00
	ATOM	237	CZ	PHE	337	31.980	-9.323	39.217	1.00	72.90
	ATOM	238	C	PHE	337	32.985	-14.013	39.245	1.00	71.38
	ATOM	239	O	PHE	337	33.336	-13.487	38.189	1.00	71.56
30	ATOM	240	N	SER	338	33.825	-14.273	40.241	1.00	71.53
	ATOM	241	CA	SER	338	35.248	-13.947	40.172	1.00	70.98
	ATOM	242	CB	SER	338	35.957	-14.487	41.414	1.00	70.43
	ATOM	243	OG	SER	338	35.547	-15.818	41.679	1.00	69.59
	ATOM	244	C	SER	338	35.931	-14.504	38.924	1.00	71.20
35	ATOM	245	O	SER	338	36.951	-13.972	38.475	1.00	71.35
	ATOM	246	N	GLU	339	35.368	-15.573	38.369	1.00	70.20
	ATOM	247	CA	GLU	339	35.930	-16.215	37.183	1.00	69.48
	ATOM	248	CB	GLU	339	35.279	-17.585	36.971	1.00	71.07
	ATOM	249	CG	GLU	339	35.996	-18.740	37.656	1.00	72.60
40	ATOM	250	CD	GLU	339	35.382	-20.089	37.318	1.00	74.26
	ATOM	251	OE1	GLU	339	34.786	-20.220	36.227	1.00	73.51
	ATOM	252	OE2	GLU	339	35.496	-21.020	38.144	1.00	76.44
	ATOM	253	C	GLU	339	35.770	-15.385	35.910	1.00	68.15
	ATOM	254	O	GLU	339	36.722	-15.216	35.144	1.00	68.99
45	ATOM	255	N	ALA	340	34.562	-14.874	35.694	1.00	64.41
	ATOM	256	CA	ALA	340	34.246	-14.083	34.507	1.00	60.69
	ATOM	257	CB	ALA	340	32.767	-13.709	34.523	1.00	61.17
	ATOM	258	C	ALA	340	35.096	-12.824	34.326	1.00	57.00
	ATOM	259	O	ALA	340	35.634	-12.270	35.287	1.00	57.46
50	ATOM	260	N	SER	341	35.215	-12.388	33.076	1.00	52.15
	ATOM	261	CA	SER	341	35.972	-11.188	32.736	1.00	46.53
	ATOM	262	CB	SER	341	36.839	-11.439	31.497	1.00	48.64
	ATOM	263	OG	SER	341	37.184	-10.226	30.846	1.00	46.48
	ATOM	264	C	SER	341	34.957	-10.087	32.444	1.00	43.52
55	ATOM	265	O	SER	341	34.090	-10.248	31.589	1.00	39.92
	ATOM	266	N	MET	342	35.052	-8.978	33.166	1.00	41.24
	ATOM	267	CA	MET	342	34.121	-7.875	32.960	1.00	42.46
	ATOM	268	CB	MET	342	34.449	-6.723	33.912	1.00	45.61
	ATOM	269	CG	MET	342	33.228	-6.089	34.560	1.00	52.39
60	ATOM	270	SD	MET	342	31.791	-7.201	34.631	1.00	57.92
	ATOM	271	CE	MET	342	31.999	-7.881	36.239	1.00	56.18

5	ATOM	272	C	MET	342	34.124	-7.365	31.516	1.00	40.22
	ATOM	273	O	MET	342	33.063	-7.121	30.938	1.00	39.23
	ATOM	274	N	MET	343	35.307	-7.204	30.930	1.00	38.72
	ATOM	275	CA	MET	343	35.395	-6.708	29.558	1.00	38.50
	ATOM	276	CB	MET	343	36.838	-6.318	29.216	1.00	41.15
10	ATOM	277	CG	MET	343	37.022	-5.749	27.804	1.00	40.31
	ATOM	278	SD	MET	343	36.032	-4.260	27.427	1.00	45.23
	ATOM	279	CE	MET	343	36.113	-3.358	28.987	1.00	40.45
	ATOM	280	C	MET	343	34.880	-7.741	28.561	1.00	35.36
	ATOM	281	O	MET	343	34.368	-7.384	27.501	1.00	35.51
15	ATOM	282	N	GLY	344	35.017	-9.020	28.902	1.00	35.53
	ATOM	283	CA	GLY	344	34.533	-10.072	28.024	1.00	33.41
	ATOM	284	C	GLY	344	33.015	-10.063	28.047	1.00	31.74
	ATOM	285	O	GLY	344	32.359	-10.233	27.019	1.00	29.58
	ATOM	286	N	LEU	345	32.459	-9.860	29.238	1.00	32.89
20	ATOM	287	CA	LEU	345	31.011	-9.804	29.415	1.00	34.95
	ATOM	288	CB	LEU	345	30.665	-9.631	30.902	1.00	37.56
	ATOM	289	CG	LEU	345	30.942	-10.774	31.883	1.00	43.03
	ATOM	290	CD1	LEU	345	30.537	-10.357	33.297	1.00	41.57
	ATOM	291	CD2	LEU	345	30.164	-11.998	31.449	1.00	42.80
25	ATOM	292	C	LEU	345	30.430	-8.614	28.633	1.00	33.71
	ATOM	293	O	LEU	345	29.479	-8.757	27.868	1.00	30.29
	ATOM	294	N	LEU	346	31.021	-7.443	28.843	1.00	30.20
	ATOM	295	CA	LEU	346	30.569	-6.217	28.193	1.00	32.00
	ATOM	296	CB	LEU	346	31.317	-5.016	28.771	1.00	28.16
30	ATOM	297	CG	LEU	346	31.091	-4.767	30.269	1.00	29.84
	ATOM	298	CD1	LEU	346	31.815	-3.498	30.668	1.00	29.98
	ATOM	299	CD2	LEU	346	29.614	-4.644	30.581	1.00	33.97
	ATOM	300	C	LEU	346	30.732	-6.250	26.682	1.00	30.70
	ATOM	301	O	LEU	346	29.869	-5.765	25.955	1.00	29.13
35	ATOM	302	N	THR	347	31.839	-6.816	26.212	1.00	30.47
	ATOM	303	CA	THR	347	32.086	-6.911	24.781	1.00	30.93
	ATOM	304	CB	THR	347	33.472	-7.501	24.497	1.00	29.97
	ATOM	305	OG1	THR	347	34.481	-6.604	24.982	1.00	35.40
	ATOM	306	CG2	THR	347	33.666	-7.707	23.004	1.00	33.58
40	ATOM	307	C	THR	347	31.036	-7.804	24.122	1.00	31.97
	ATOM	308	O	THR	347	30.516	-7.486	23.049	1.00	30.75
	ATOM	309	N	ASN	348	30.737	-8.926	24.768	1.00	29.31
	ATOM	310	CA	ASN	348	29.757	-9.868	24.242	1.00	32.63
	ATOM	311	CB	ASN	348	29.767	-11.161	25.065	1.00	31.64
45	ATOM	312	CG	ASN	348	28.646	-12.117	24.662	1.00	39.14
	ATOM	313	OD1	ASN	348	27.549	-12.078	25.220	1.00	41.91
	ATOM	314	ND2	ASN	348	28.920	-12.970	23.683	1.00	42.05
	ATOM	315	C	ASN	348	28.361	-9.251	24.262	1.00	29.02
	ATOM	316	O	ASN	348	27.558	-9.477	23.353	1.00	32.76
50	ATOM	317	N	LEU	349	28.078	-8.467	25.298	1.00	28.74
	ATOM	318	CA	LEU	349	26.782	-7.811	25.421	1.00	28.58
	ATOM	319	CB	LEU	349	26.650	-7.148	26.795	1.00	26.56
	ATOM	320	CG	LEU	349	25.376	-6.328	27.050	1.00	33.67
	ATOM	321	CD1	LEU	349	24.140	-7.199	26.840	1.00	28.82
55	ATOM	322	CD2	LEU	349	25.392	-5.779	28.471	1.00	33.11
	ATOM	323	C	LEU	349	26.638	-6.762	24.319	1.00	28.07
	ATOM	324	O	LEU	349	25.616	-6.703	23.629	1.00	25.22
	ATOM	325	N	ALA	350	27.675	-5.941	24.157	1.00	28.50
	ATOM	326	CA	ALA	350	27.668	-4.886	23.148	1.00	28.46
60	ATOM	327	CB	ALA	350	28.972	-4.094	23.209	1.00	28.12
	ATOM	328	C	ALA	350	27.468	-5.461	21.750	1.00	28.75

5	ATOM	329	O	ALA	350	26.649	-4.958	20.983	1.00	30.90
	ATOM	330	N	ASP	351	28.213	-6.509	21.420	1.00	27.20
	ATOM	331	CA	ASP	351	28.093	-7.143	20.112	1.00	29.75
	ATOM	332	CB	ASP	351	29.036	-8.345	20.010	1.00	34.16
	ATOM	333	CG	ASP	351	30.498	-7.940	19.978	1.00	37.50
10	ATOM	334	OD1	ASP	351	31.354	-8.831	20.148	1.00	37.55
	ATOM	335	OD2	ASP	351	30.789	-6.738	19.784	1.00	35.50
	ATOM	336	C	ASP	351	26.661	-7.600	19.813	1.00	30.52
	ATOM	337	O	ASP	351	26.193	-7.458	18.687	1.00	27.77
	ATOM	338	N	ARG	352	25.968	-8.150	20.811	1.00	27.18
15	ATOM	339	CA	ARG	352	24.593	-8.602	20.605	1.00	26.21
	ATOM	340	CB	ARG	352	24.148	-9.534	21.752	1.00	26.52
	ATOM	341	CG	ARG	352	24.567	-10.991	21.532	1.00	31.03
	ATOM	342	CD	ARG	352	24.128	-11.911	22.666	1.00	29.80
	ATOM	343	NE	ARG	352	24.898	-11.675	23.879	1.00	30.44
20	ATOM	344	CZ	ARG	352	24.364	-11.363	25.054	1.00	31.68
	ATOM	345	NH1	ARG	352	23.050	-11.251	25.177	1.00	31.18
	ATOM	346	NH2	ARG	352	25.144	-11.148	26.104	1.00	32.03
	ATOM	347	C	ARG	352	23.642	-7.411	20.502	1.00	27.16
	ATOM	348	O	ARG	352	22.702	-7.426	19.708	1.00	26.65
25	ATOM	349	N	GLU	353	23.896	-6.370	21.291	1.00	24.30
	ATOM	350	CA	GLU	353	23.045	-5.178	21.261	1.00	26.39
	ATOM	351	CB	GLU	353	23.461	-4.204	22.365	1.00	24.91
	ATOM	352	CG	GLU	353	23.147	-4.669	23.771	1.00	27.93
	ATOM	353	CD	GLU	353	23.425	-3.587	24.795	1.00	30.71
30	ATOM	354	OE1	GLU	353	24.564	-3.534	25.304	1.00	30.09
	ATOM	355	OE2	GLU	353	22.506	-2.789	25.085	1.00	30.53
	ATOM	356	C	GLU	353	23.131	-4.456	19.920	1.00	24.27
	ATOM	357	O	GLU	353	22.169	-3.826	19.467	1.00	28.71
	ATOM	358	N	LEU	354	24.296	-4.540	19.293	1.00	26.61
35	ATOM	359	CA	LEU	354	24.522	-3.872	18.017	1.00	26.62
	ATOM	360	CB	LEU	354	25.952	-4.121	17.543	1.00	26.36
	ATOM	361	CG	LEU	354	26.372	-3.257	16.351	1.00	29.24
	ATOM	362	CD1	LEU	354	26.243	-1.774	16.722	1.00	26.59
	ATOM	363	CD2	LEU	354	27.794	-3.607	15.962	1.00	28.88
40	ATOM	364	C	LEU	354	23.559	-4.300	16.926	1.00	27.72
	ATOM	365	O	LEU	354	23.074	-3.475	16.152	1.00	24.00
	ATOM	366	N	VAL	355	23.291	-5.598	16.854	1.00	28.82
	ATOM	367	CA	VAL	355	22.386	-6.125	15.844	1.00	29.45
	ATOM	368	CB	VAL	355	22.259	-7.655	15.975	1.00	31.76
45	ATOM	369	CG1	VAL	355	21.423	-8.205	14.834	1.00	33.55
	ATOM	370	CG2	VAL	355	23.649	-8.282	15.998	1.00	31.36
	ATOM	371	C	VAL	355	21.020	-5.499	16.035	1.00	27.71
	ATOM	372	O	VAL	355	20.382	-5.039	15.080	1.00	29.61
	ATOM	373	N	HIS	356	20.580	-5.473	17.288	1.00	27.76
50	ATOM	374	CA	HIS	356	19.291	-4.906	17.627	1.00	28.35
	ATOM	375	CB	HIS	356	18.936	-5.231	19.079	1.00	31.12
	ATOM	376	CG	HIS	356	18.602	-6.675	19.307	1.00	35.93
	ATOM	377	CD2	HIS	356	19.352	-7.700	19.779	1.00	33.95
	ATOM	378	ND1	HIS	356	17.363	-7.208	19.018	1.00	36.62
55	ATOM	379	CE1	HIS	356	17.364	-8.499	19.304	1.00	33.33
	ATOM	380	NE2	HIS	356	18.559	-8.823	19.767	1.00	32.16
	ATOM	381	C	HIS	356	19.300	-3.398	17.412	1.00	28.25
	ATOM	382	O	HIS	356	18.272	-2.812	17.100	1.00	28.99
	ATOM	383	N	MET	357	20.457	-2.765	17.574	1.00	25.31
60	ATOM	384	CA	MET	357	20.526	-1.322	17.369	1.00	24.63
	ATOM	385	CB	MET	357	21.902	-0.789	17.766	1.00	23.61

5	ATOM	386	CG	MET	357	22.011	0.736	17.699	1.00	24.66
	ATOM	387	SD	MET	357	23.732	1.290	17.859	1.00	27.30
	ATOM	388	CE	MET	357	24.140	0.672	19.514	1.00	23.62
	ATOM	389	C	MET	357	20.256	-1.011	15.898	1.00	24.83
	ATOM	390	O	MET	357	19.619	-0.003	15.569	1.00	26.78
10	ATOM	391	N	ILE	358	20.757	-1.874	15.020	1.00	26.25
	ATOM	392	CA	ILE	358	20.553	-1.721	13.576	1.00	30.33
	ATOM	393	CB	ILE	358	21.204	-2.888	12.789	1.00	33.86
	ATOM	394	CG2	ILE	358	20.759	-2.860	11.334	1.00	33.68
	ATOM	395	CG1	ILE	358	22.728	-2.799	12.874	1.00	36.89
15	ATOM	396	CD1	ILE	358	23.299	-1.469	12.451	1.00	39.10
	ATOM	397	C	ILE	358	19.055	-1.721	13.310	1.00	32.20
	ATOM	398	O	ILE	358	18.519	-0.817	12.662	1.00	32.02
	ATOM	399	N	ASN	359	18.379	-2.748	13.814	1.00	33.12
	ATOM	400	CA	ASN	359	16.945	-2.861	13.638	1.00	33.35
20	ATOM	401	CB	ASN	359	16.434	-4.101	14.363	1.00	37.59
	ATOM	402	CG	ASN	359	16.739	-5.374	13.627	1.00	44.38
	ATOM	403	OD1	ASN	359	17.045	-5.329	12.437	1.00	47.35
	ATOM	404	ND2	ASN	359	16.673	-6.508	14.320	1.00	42.48
	ATOM	405	C	ASN	359	16.224	-1.634	14.149	1.00	32.74
25	ATOM	406	O	ASN	359	15.261	-1.163	13.530	1.00	31.39
	ATOM	407	N	TRP	360	16.706	-1.104	15.264	1.00	27.92
	ATOM	408	CA	TRP	360	16.102	0.087	15.842	1.00	29.47
	ATOM	409	CB	TRP	360	16.703	0.347	17.228	1.00	27.66
	ATOM	410	CG	TRP	360	16.522	1.747	17.707	1.00	30.40
30	ATOM	411	CD2	TRP	360	17.493	2.801	17.657	1.00	27.54
	ATOM	412	CE2	TRP	360	16.888	3.954	18.204	1.00	29.42
	ATOM	413	CE3	TRP	360	18.819	2.883	17.205	1.00	28.37
	ATOM	414	CD1	TRP	360	15.399	2.284	18.264	1.00	27.75
	ATOM	415	NE1	TRP	360	15.609	3.611	18.566	1.00	30.84
35	ATOM	416	CZ2	TRP	360	17.558	5.180	18.310	1.00	27.74
	ATOM	417	CZ3	TRP	360	19.488	4.106	17.309	1.00	24.49
	ATOM	418	CH2	TRP	360	18.853	5.232	17.858	1.00	25.09
	ATOM	419	C	TRP	360	16.312	1.296	14.926	1.00	27.90
	ATOM	420	O	TRP	360	15.360	2.002	14.581	1.00	28.83
40	ATOM	421	N	ALA	361	17.559	1.520	14.523	1.00	28.25
	ATOM	422	CA	ALA	361	17.894	2.637	13.645	1.00	29.20
	ATOM	423	CB	ALA	361	19.346	2.539	13.220	1.00	28.89
	ATOM	424	C	ALA	361	17.006	2.685	12.403	1.00	31.08
	ATOM	425	O	ALA	361	16.531	3.746	12.011	1.00	31.30
45	ATOM	426	N	LYS	362	16.795	1.526	11.783	1.00	30.93
	ATOM	427	CA	LYS	362	15.981	1.443	10.581	1.00	34.15
	ATOM	428	CB	LYS	362	16.012	0.016	10.023	1.00	33.67
	ATOM	429	CG	LYS	362	17.252	-0.281	9.198	1.00	39.40
	ATOM	430	CD	LYS	362	17.547	-1.774	9.136	1.00	43.60
50	ATOM	431	CE	LYS	362	18.852	-2.046	8.389	1.00	47.06
	ATOM	432	NZ	LYS	362	19.178	-3.507	8.288	1.00	50.34
	ATOM	433	C	LYS	362	14.545	1.872	10.815	1.00	35.81
	ATOM	434	O	LYS	362	13.821	2.168	9.859	1.00	37.95
	ATOM	435	N	ARG	363	14.134	1.921	12.079	1.00	34.23
55	ATOM	436	CA	ARG	363	12.770	2.313	12.409	1.00	36.04
	ATOM	437	CB	ARG	363	12.178	1.307	13.391	1.00	36.71
	ATOM	438	CG	ARG	363	12.169	-0.110	12.827	1.00	40.36
	ATOM	439	CD	ARG	363	11.468	-1.086	13.746	1.00	42.17
	ATOM	440	NE	ARG	363	10.161	-0.586	14.158	1.00	45.19
60	ATOM	441	CZ	ARG	363	9.314	-1.262	14.929	1.00	49.41
	ATOM	442	NH1	ARG	363	9.642	-2.467	15.374	1.00	48.02

5	ATOM	443	NH2	ARG	363	8.143	-0.729	15.261	1.00	51.54
	ATOM	444	C	ARG	363	12.654	3.743	12.943	1.00	37.40
	ATOM	445	O	ARG	363	11.567	4.199	13.303	1.00	38.22
	ATOM	446	N	VAL	364	13.785	4.442	13.002	1.00	35.66
	ATOM	447	CA	VAL	364	13.804	5.836	13.431	1.00	34.06
10	ATOM	448	CB	VAL	364	15.231	6.271	13.827	1.00	33.87
	ATOM	449	CG1	VAL	364	15.293	7.779	13.995	1.00	31.08
	ATOM	450	CG2	VAL	364	15.641	5.571	15.113	1.00	31.30
	ATOM	451	C	VAL	364	13.360	6.591	12.171	1.00	33.19
	ATOM	452	O	VAL	364	14.028	6.531	11.146	1.00	33.04
15	ATOM	453	N	PRO	365	12.225	7.310	12.234	1.00	34.69
	ATOM	454	CD	PRO	365	11.359	7.492	13.413	1.00	34.19
	ATOM	455	CA	PRO	365	11.724	8.050	11.069	1.00	35.96
	ATOM	456	CB	PRO	365	10.608	8.918	11.645	1.00	36.59
	ATOM	457	CG	PRO	365	10.135	8.157	12.842	1.00	39.59
20	ATOM	458	C	PRO	365	12.756	8.878	10.321	1.00	37.19
	ATOM	459	O	PRO	365	13.430	9.726	10.907	1.00	40.29
	ATOM	460	N	GLY	366	12.878	8.624	9.023	1.00	34.78
	ATOM	461	CA	GLY	366	13.816	9.371	8.212	1.00	33.54
	ATOM	462	C	GLY	366	15.168	8.722	8.007	1.00	34.26
25	ATOM	463	O	GLY	366	15.858	9.035	7.034	1.00	37.15
	ATOM	464	N	PHE	367	15.554	7.814	8.901	1.00	33.13
	ATOM	465	CA	PHE	367	16.860	7.164	8.787	1.00	32.04
	ATOM	466	CB	PHE	367	17.138	6.291	10.016	1.00	30.22
	ATOM	467	CG	PHE	367	18.544	5.773	10.080	1.00	30.60
30	ATOM	468	CD1	PHE	367	18.827	4.446	9.751	1.00	31.94
	ATOM	469	CD2	PHE	367	19.589	6.601	10.485	1.00	29.20
	ATOM	470	CE1	PHE	367	20.133	3.950	9.828	1.00	28.30
	ATOM	471	CE2	PHE	367	20.896	6.122	10.568	1.00	28.12
	ATOM	472	CZ	PHE	367	21.171	4.791	10.240	1.00	25.41
35	ATOM	473	C	PHE	367	17.033	6.333	7.524	1.00	31.46
	ATOM	474	O	PHE	367	18.073	6.405	6.883	1.00	32.30
	ATOM	475	N	VAL	368	16.027	5.541	7.165	1.00	35.20
	ATOM	476	CA	VAL	368	16.123	4.718	5.959	1.00	38.98
	ATOM	477	CB	VAL	368	15.076	3.584	5.945	1.00	40.61
40	ATOM	478	CG1	VAL	368	15.543	2.447	6.843	1.00	41.48
	ATOM	479	CG2	VAL	368	13.717	4.113	6.390	1.00	41.60
	ATOM	480	C	VAL	368	15.965	5.523	4.673	1.00	40.06
	ATOM	481	O	VAL	368	16.156	4.992	3.579	1.00	41.66
	ATOM	482	N	ASP	369	15.608	6.798	4.798	1.00	38.65
45	ATOM	483	CA	ASP	369	15.465	7.646	3.621	1.00	37.15
	ATOM	484	CB	ASP	369	14.700	8.929	3.954	1.00	39.89
	ATOM	485	CG	ASP	369	13.254	8.671	4.302	1.00	45.59
	ATOM	486	OD1	ASP	369	12.686	7.672	3.806	1.00	46.34
	ATOM	487	OD2	ASP	369	12.681	9.472	5.074	1.00	49.13
50	ATOM	488	C	ASP	369	16.855	8.010	3.136	1.00	34.91
	ATOM	489	O	ASP	369	17.038	8.431	1.995	1.00	34.25
	ATOM	490	N	LEU	370	17.838	7.841	4.016	1.00	31.76
	ATOM	491	CA	LEU	370	19.229	8.153	3.705	1.00	28.08
	ATOM	492	CB	LEU	370	20.020	8.339	5.003	1.00	28.81
55	ATOM	493	CG	LEU	370	19.523	9.395	6.000	1.00	28.74
	ATOM	494	CD1	LEU	370	20.315	9.275	7.299	1.00	30.81
	ATOM	495	CD2	LEU	370	19.693	10.792	5.404	1.00	29.77
	ATOM	496	C	LEU	370	19.884	7.043	2.893	1.00	31.25
	ATOM	497	O	LEU	370	19.341	5.943	2.784	1.00	31.78
60	ATOM	498	N	THR	371	21.052	7.333	2.331	1.00	28.86
	ATOM	499	CA	THR	371	21.793	6.336	1.569	1.00	32.90

5	ATOM	500	CB	THR	371	22.979	6.944	0.818	1.00	33.44
	ATOM	501	OG1	THR	371	23.880	7.523	1.766	1.00	34.59
	ATOM	502	CG2	THR	371	22.514	8.002	-0.178	1.00	32.63
	ATOM	503	C	THR	371	22.373	5.315	2.539	1.00	35.31
	ATOM	504	O	THR	371	22.536	5.591	3.733	1.00	31.27
10	ATOM	505	N	LEU	372	22.702	4.141	2.015	1.00	34.34
	ATOM	506	CA	LEU	372	23.273	3.073	2.822	1.00	35.46
	ATOM	507	CB	LEU	372	23.518	1.841	1.944	1.00	37.73
	ATOM	508	CG	LEU	372	24.362	0.704	2.515	1.00	42.43
	ATOM	509	CD1	LEU	372	23.690	0.145	3.757	1.00	45.60
15	ATOM	510	CD2	LEU	372	24.534	-0.383	1.455	1.00	44.29
	ATOM	511	C	LEU	372	24.587	3.548	3.444	1.00	36.95
	ATOM	512	O	LEU	372	24.813	3.374	4.643	1.00	35.57
	ATOM	513	N	HIS	373	25.442	4.159	2.627	1.00	35.68
	ATOM	514	CA	HIS	373	26.729	4.656	3.099	1.00	36.60
20	ATOM	515	CB	HIS	373	27.506	5.282	1.935	1.00	44.01
	ATOM	516	CG	HIS	373	28.538	6.280	2.360	1.00	50.69
	ATOM	517	CD2	HIS	373	29.857	6.138	2.636	1.00	54.69
	ATOM	518	ND1	HIS	373	28.246	7.613	2.561	1.00	53.77
	ATOM	519	CE1	HIS	373	29.339	8.248	2.945	1.00	57.09
25	ATOM	520	NE2	HIS	373	30.331	7.376	2.999	1.00	57.23
	ATOM	521	C	HIS	373	26.575	5.669	4.244	1.00	36.22
	ATOM	522	O	HIS	373	27.350	5.650	5.201	1.00	33.05
	ATOM	523	N	ASP	374	25.580	6.549	4.148	1.00	32.03
	ATOM	524	CA	ASP	374	25.342	7.541	5.196	1.00	30.76
30	ATOM	525	CB	ASP	374	24.354	8.603	4.713	1.00	30.12
	ATOM	526	CG	ASP	374	25.018	9.672	3.860	1.00	35.83
	ATOM	527	OD1	ASP	374	26.264	9.744	3.842	1.00	34.39
	ATOM	528	OD2	ASP	374	24.291	10.440	3.199	1.00	35.39
	ATOM	529	C	ASP	374	24.805	6.876	6.472	1.00	30.33
35	ATOM	530	O	ASP	374	25.152	7.275	7.587	1.00	27.04
	ATOM	531	N	GLN	375	23.944	5.877	6.309	1.00	25.71
	ATOM	532	CA	GLN	375	23.403	5.157	7.454	1.00	26.68
	ATOM	533	CB	GLN	375	22.424	4.077	6.993	1.00	29.70
	ATOM	534	CG	GLN	375	21.101	4.616	6.484	1.00	29.16
40	ATOM	535	CD	GLN	375	20.219	3.514	5.940	1.00	35.87
	ATOM	536	OE1	GLN	375	20.155	2.426	6.510	1.00	30.97
	ATOM	537	NE2	GLN	375	19.541	3.785	4.827	1.00	34.51
	ATOM	538	C	GLN	375	24.556	4.502	8.214	1.00	25.51
	ATOM	539	O	GLN	375	24.585	4.513	9.442	1.00	28.14
45	ATOM	540	N	VAL	376	25.504	3.938	7.475	1.00	26.62
	ATOM	541	CA	VAL	376	26.659	3.281	8.071	1.00	29.24
	ATOM	542	CB	VAL	376	27.531	2.597	7.003	1.00	29.66
	ATOM	543	CG1	VAL	376	28.812	2.071	7.635	1.00	28.29
	ATOM	544	CG2	VAL	376	26.745	1.469	6.341	1.00	29.90
50	ATOM	545	C	VAL	376	27.526	4.285	8.821	1.00	30.87
	ATOM	546	O	VAL	376	27.953	4.029	9.948	1.00	30.09
	ATOM	547	N	HIS	377	27.785	5.428	8.191	1.00	28.05
	ATOM	548	CA	HIS	377	28.602	6.457	8.814	1.00	28.68
	ATOM	549	CB	HIS	377	28.792	7.639	7.864	1.00	30.26
55	ATOM	550	CG	HIS	377	29.508	8.791	8.488	1.00	33.89
	ATOM	551	CD2	HIS	377	29.073	10.017	8.863	1.00	34.99
	ATOM	552	ND1	HIS	377	30.846	8.740	8.823	1.00	37.01
	ATOM	553	CE1	HIS	377	31.201	9.884	9.377	1.00	34.79
	ATOM	554	NE2	HIS	377	30.144	10.677	9.413	1.00	34.95
60	ATOM	555	C	HIS	377	27.983	6.954	10.114	1.00	25.13
	ATOM	556	O	HIS	377	28.677	7.102	11.115	1.00	25.93

5	ATOM	557	N	LEU	378	26.678	7.206	10.107	1.00	24.58
	ATOM	558	CA	LEU	378	26.015	7.695	11.315	1.00	26.40
	ATOM	559	CB	LEU	378	24.542	8.001	11.027	1.00	26.29
	ATOM	560	CG	LEU	378	24.291	9.180	10.073	1.00	28.06
	ATOM	561	CD1	LEU	378	22.778	9.353	9.869	1.00	27.66
10	ATOM	562	CD2	LEU	378	24.911	10.458	10.642	1.00	30.08
	ATOM	563	C	LEU	378	26.120	6.695	12.459	1.00	28.55
	ATOM	564	O	LEU	378	26.379	7.075	13.605	1.00	24.76
	ATOM	565	N	LEU	379	25.919	5.414	12.153	1.00	24.29
	ATOM	566	CA	LEU	379	26.000	4.388	13.182	1.00	27.03
15	ATOM	567	CB	LEU	379	25.401	3.073	12.667	1.00	28.53
	ATOM	568	CG	LEU	379	23.875	3.023	12.845	1.00	30.29
	ATOM	569	CD1	LEU	379	23.248	1.943	11.963	1.00	33.04
	ATOM	570	CD2	LEU	379	23.563	2.759	14.312	1.00	29.45
	ATOM	571	C	LEU	379	27.430	4.176	13.670	1.00	27.18
20	ATOM	572	O	LEU	379	27.653	3.979	14.866	1.00	25.95
	ATOM	573	N	GLU	380	28.402	4.236	12.762	1.00	25.86
	ATOM	574	CA	GLU	380	29.786	4.054	13.173	1.00	27.58
	ATOM	575	CB	GLU	380	30.730	4.036	11.968	1.00	30.36
	ATOM	576	CG	GLU	380	32.172	3.785	12.380	1.00	37.98
25	ATOM	577	CD	GLU	380	33.080	3.471	11.210	1.00	45.23
	ATOM	578	OE1	GLU	380	32.869	4.048	10.120	1.00	42.99
	ATOM	579	OE2	GLU	380	34.004	2.646	11.386	1.00	45.79
	ATOM	580	C	GLU	380	30.218	5.159	14.133	1.00	27.50
	ATOM	581	O	GLU	380	31.056	4.937	15.010	1.00	26.67
30	ATOM	582	N	ACYS	381	29.637	6.339	13.965	0.75	24.89
	ATOM	583	N	BCYS	381	29.645	6.352	13.980	0.25	25.79
	ATOM	584	CA	ACYS	381	29.969	7.466	14.826	0.75	24.12
	ATOM	585	CA	BCYS	381	29.993	7.481	14.847	0.25	24.86
	ATOM	586	CB	ACYS	381	29.621	8.781	14.122	0.75	25.96
35	ATOM	587	CB	BCYS	381	29.766	8.814	14.115	0.25	25.62
	ATOM	588	SG	ACYS	381	30.698	9.192	12.732	0.75	31.63
	ATOM	589	SG	BCYS	381	30.227	10.312	15.059	0.25	25.40
	ATOM	590	C	ACYS	381	29.237	7.422	16.162	0.75	22.07
	ATOM	591	C	BCYS	381	29.211	7.498	16.159	0.25	23.97
40	ATOM	592	O	ACYS	381	29.812	7.730	17.206	0.75	21.97
	ATOM	593	O	BCYS	381	29.724	7.940	17.187	0.25	23.99
	ATOM	594	N	ALA	382	27.974	7.012	16.128	1.00	23.41
	ATOM	595	CA	ALA	382	27.140	7.015	17.318	1.00	22.83
	ATOM	596	CB	ALA	382	25.785	7.587	16.948	1.00	25.50
45	ATOM	597	C	ALA	382	26.913	5.755	18.131	1.00	25.39
	ATOM	598	O	ALA	382	26.374	5.837	19.234	1.00	23.09
	ATOM	599	N	TRP	383	27.311	4.602	17.615	1.00	25.98
	ATOM	600	CA	TRP	383	27.026	3.354	18.318	1.00	23.80
	ATOM	601	CB	TRP	383	27.669	2.172	17.580	1.00	22.52
50	ATOM	602	CG	TRP	383	29.130	2.054	17.762	1.00	24.42
	ATOM	603	CD2	TRP	383	29.797	1.347	18.803	1.00	27.31
	ATOM	604	CE2	TRP	383	31.182	1.484	18.579	1.00	28.24
	ATOM	605	CE3	TRP	383	29.360	0.609	19.912	1.00	27.37
	ATOM	606	CD1	TRP	383	30.102	2.578	16.965	1.00	24.58
55	ATOM	607	NE1	TRP	383	31.342	2.239	17.446	1.00	27.35
	ATOM	608	CZ2	TRP	383	32.133	0.909	19.420	1.00	28.76
	ATOM	609	CZ3	TRP	383	30.305	0.039	20.745	1.00	28.09
	ATOM	610	CH2	TRP	383	31.674	0.191	20.496	1.00	29.77
	ATOM	611	C	TRP	383	27.356	3.309	19.802	1.00	23.54
60	ATOM	612	O	TRP	383	26.526	2.866	20.584	1.00	22.90
	ATOM	613	N	LEU	384	28.542	3.765	20.211	1.00	20.37

5	ATOM	614	CA	LEU	384	28.864	3.713	21.640	1.00	22.41
	ATOM	615	CB	LEU	384	30.369	3.890	21.883	1.00	24.98
	ATOM	616	CG	LEU	384	30.824	3.645	23.336	1.00	27.33
	ATOM	617	CD1	LEU	384	30.273	2.305	23.853	1.00	29.71
	ATOM	618	CD2	LEU	384	32.336	3.648	23.398	1.00	26.07
10	ATOM	619	C	LEU	384	28.075	4.732	22.453	1.00	19.44
	ATOM	620	O	LEU	384	27.706	4.458	23.595	1.00	23.24
	ATOM	621	N	GLU	385	27.807	5.909	21.885	1.00	20.80
	ATOM	622	CA	GLU	385	27.011	6.895	22.612	1.00	21.32
	ATOM	623	CB	GLU	385	26.861	8.177	21.797	1.00	21.91
15	ATOM	624	CG	GLU	385	28.115	9.020	21.705	1.00	21.61
	ATOM	625	CD	GLU	385	27.882	10.256	20.860	1.00	29.53
	ATOM	626	OE1	GLU	385	27.374	11.256	21.401	1.00	30.54
	ATOM	627	OE2	GLU	385	28.188	10.219	19.658	1.00	29.97
	ATOM	628	C	GLU	385	25.616	6.292	22.836	1.00	22.26
20	ATOM	629	O	GLU	385	25.022	6.438	23.902	1.00	22.26
	ATOM	630	N	ILE	386	25.101	5.617	21.812	1.00	22.03
	ATOM	631	CA	ILE	386	23.779	4.995	21.896	1.00	22.74
	ATOM	632	CB	ILE	386	23.328	4.455	20.498	1.00	22.88
	ATOM	633	CG2	ILE	386	22.009	3.647	20.618	1.00	23.85
25	ATOM	634	CG1	ILE	386	23.085	5.651	19.561	1.00	25.05
	ATOM	635	CD1	ILE	386	22.994	5.297	18.078	1.00	26.42
	ATOM	636	C	ILE	386	23.766	3.897	22.961	1.00	22.50
	ATOM	637	O	ILE	386	22.823	3.818	23.746	1.00	24.75
	ATOM	638	N	LEU	387	24.810	3.071	23.020	1.00	22.25
30	ATOM	639	CA	LEU	387	24.868	2.030	24.051	1.00	22.95
	ATOM	640	CB	LEU	387	26.096	1.132	23.864	1.00	24.61
	ATOM	641	CG	LEU	387	26.070	0.194	22.654	1.00	23.21
	ATOM	642	CD1	LEU	387	27.297	-0.709	22.705	1.00	25.36
	ATOM	643	CD2	LEU	387	24.791	-0.631	22.652	1.00	26.29
35	ATOM	644	C	LEU	387	24.944	2.660	25.438	1.00	26.22
	ATOM	645	O	LEU	387	24.287	2.204	26.386	1.00	23.55
	ATOM	646	N	MET	388	25.751	3.713	25.554	1.00	23.92
	ATOM	647	CA	MET	388	25.924	4.385	26.835	1.00	24.26
	ATOM	648	CB	MET	388	27.088	5.378	26.761	1.00	23.87
40	ATOM	649	CG	MET	388	28.440	4.722	26.743	1.00	24.08
	ATOM	650	SD	MET	388	29.726	5.992	26.736	1.00	27.70
	ATOM	651	CE	MET	388	31.139	5.041	27.078	1.00	21.74
	ATOM	652	C	MET	388	24.660	5.094	27.321	1.00	23.33
	ATOM	653	O	MET	388	24.341	5.026	28.505	1.00	25.58
45	ATOM	654	N	ILE	389	23.935	5.775	26.436	1.00	24.62
	ATOM	655	CA	ILE	389	22.729	6.440	26.905	1.00	24.03
	ATOM	656	CB	ILE	389	22.132	7.439	25.852	1.00	27.01
	ATOM	657	CG2	ILE	389	21.413	6.705	24.706	1.00	23.98
	ATOM	658	CG1	ILE	389	21.185	8.402	26.584	1.00	25.49
50	ATOM	659	CD1	ILE	389	20.431	9.383	25.683	1.00	25.45
	ATOM	660	C	ILE	389	21.694	5.401	27.349	1.00	26.54
	ATOM	661	O	ILE	389	20.938	5.631	28.294	1.00	22.58
	ATOM	662	N	GLY	390	21.679	4.247	26.687	1.00	27.14
	ATOM	663	CA	GLY	390	20.753	3.201	27.090	1.00	28.42
55	ATOM	664	C	GLY	390	21.133	2.719	28.482	1.00	29.67
	ATOM	665	O	GLY	390	20.275	2.521	29.348	1.00	29.21
	ATOM	666	N	LEU	391	22.433	2.547	28.699	1.00	26.06
	ATOM	667	CA	LEU	391	22.955	2.091	29.983	1.00	29.23
	ATOM	668	CB	LEU	391	24.476	1.937	29.899	1.00	28.37
60	ATOM	669	CG	LEU	391	25.206	1.656	31.210	1.00	30.81
	ATOM	670	CD1	LEU	391	24.717	0.332	31.793	1.00	25.73



5	ATOM	671	CD2	LEU	391	26.709	1.619	30.958	1.00	25.25
	ATOM	672	C	LEU	391	22.603	3.070	31.104	1.00	30.84
	ATOM	673	O	LEU	391	22.156	2.669	32.186	1.00	29.19
	ATOM	674	N	VAL	392	22.817	4.355	30.850	1.00	28.91
	ATOM	675	CA	VAL	392	22.506	5.369	31.851	1.00	28.86
10	ATOM	676	CB	VAL	392	22.923	6.770	31.353	1.00	30.08
	ATOM	677	CG1	VAL	392	22.329	7.854	32.237	1.00	32.32
	ATOM	678	CG2	VAL	392	24.442	6.870	31.372	1.00	28.52
	ATOM	679	C	VAL	392	21.013	5.327	32.165	1.00	28.42
	ATOM	680	O	VAL	392	20.621	5.345	33.327	1.00	30.38
15	ATOM	681	N	TRP	393	20.191	5.241	31.125	1.00	28.23
	ATOM	682	CA	TRP	393	18.732	5.186	31.280	1.00	29.70
	ATOM	683	CB	TRP	393	18.066	5.046	29.906	1.00	30.09
	ATOM	684	CG	TRP	393	16.605	4.670	29.953	1.00	33.50
	ATOM	685	CD2	TRP	393	15.516	5.499	30.369	1.00	31.76
20	ATOM	686	CE2	TRP	393	14.336	4.725	30.264	1.00	38.11
	ATOM	687	CE3	TRP	393	15.419	6.821	30.824	1.00	32.56
	ATOM	688	CD1	TRP	393	16.057	3.459	29.618	1.00	34.31
	ATOM	689	NE1	TRP	393	14.696	3.486	29.801	1.00	34.36
	ATOM	690	CZ2	TRP	393	13.073	5.233	30.597	1.00	37.93
25	ATOM	691	CZ3	TRP	393	14.162	7.326	31.155	1.00	35.24
	ATOM	692	CH2	TRP	393	13.007	6.531	31.039	1.00	37.77
	ATOM	693	C	TRP	393	18.256	4.051	32.191	1.00	32.07
	ATOM	694	O	TRP	393	17.460	4.275	33.109	1.00	32.12
	ATOM	695	N	ARG	394	18.738	2.837	31.957	1.00	31.90
30	ATOM	696	CA	ARG	394	18.288	1.729	32.787	1.00	36.63
	ATOM	697	CB	ARG	394	18.492	0.389	32.065	1.00	36.41
	ATOM	698	CG	ARG	394	19.914	0.009	31.764	1.00	36.50
	ATOM	699	CD	ARG	394	19.929	-1.132	30.748	1.00	36.34
	ATOM	700	NE	ARG	394	21.282	-1.561	30.417	1.00	33.97
35	ATOM	701	CZ	ARG	394	21.864	-1.350	29.239	1.00	31.61
	ATOM	702	NH1	ARG	394	21.208	-0.715	28.281	1.00	32.42
	ATOM	703	NH2	ARG	394	23.098	-1.784	29.022	1.00	29.81
	ATOM	704	C	ARG	394	18.911	1.697	34.180	1.00	36.69
	ATOM	705	O	ARG	394	18.445	0.966	35.048	1.00	37.07
40	ATOM	706	N	SER	395	19.954	2.492	34.395	1.00	33.63
	ATOM	707	CA	SER	395	20.603	2.564	35.701	1.00	35.69
	ATOM	708	CB	SER	395	22.112	2.784	35.540	1.00	32.94
	ATOM	709	OG	SER	395	22.696	1.811	34.688	1.00	32.37
	ATOM	710	C	SER	395	20.010	3.713	36.531	1.00	36.44
45	ATOM	711	O	SER	395	20.389	3.916	37.687	1.00	38.68
	ATOM	712	N	MET	396	19.076	4.449	35.937	1.00	36.46
	ATOM	713	CA	MET	396	18.431	5.588	36.589	1.00	43.08
	ATOM	714	CB	MET	396	17.275	6.104	35.725	1.00	43.87
	ATOM	715	CG	MET	396	17.481	7.507	35.176	1.00	46.18
50	ATOM	716	SD	MET	396	15.962	8.278	34.581	1.00	49.58
	ATOM	717	CE	MET	396	14.988	8.298	36.065	1.00	53.58
	ATOM	718	C	MET	396	17.906	5.303	37.992	1.00	46.18
	ATOM	719	O	MET	396	18.125	6.089	38.913	1.00	46.34
	ATOM	720	N	GLU	397	17.215	4.180	38.152	1.00	49.39
55	ATOM	721	CA	GLU	397	16.645	3.821	39.444	1.00	52.12
	ATOM	722	CB	GLU	397	15.296	3.130	39.246	1.00	55.34
	ATOM	723	CG	GLU	397	14.166	4.073	38.873	1.00	58.86
	ATOM	724	CD	GLU	397	13.195	3.448	37.891	1.00	63.28
	ATOM	725	OE1	GLU	397	13.660	2.925	36.854	1.00	64.68
60	ATOM	726	OE2	GLU	397	11.972	3.475	38.155	1.00	65.39
	ATOM	727	C	GLU	397	17.548	2.933	40.283	1.00	52.75

5	ATOM	728	O	GLU	397	17.071	2.187	41.139	1.00	53.96
	ATOM	729	N	HIS	398	18.851	3.014	40.040	1.00	50.25
	ATOM	730	CA	HIS	398	19.813	2.220	40.792	1.00	49.34
	ATOM	731	CB	HIS	398	20.271	1.018	39.963	1.00	52.04
	ATOM	732	CG	HIS	398	19.187	0.017	39.721	1.00	53.95
10	ATOM	733	CD2	HIS	398	18.750	-1.022	40.472	1.00	53.92
	ATOM	734	ND1	HIS	398	18.374	0.054	38.608	1.00	55.91
	ATOM	735	CE1	HIS	398	17.482	-0.917	38.685	1.00	55.53
	ATOM	736	NE2	HIS	398	17.688	-1.585	39.806	1.00	55.81
	ATOM	737	C	HIS	398	20.999	3.084	41.196	1.00	47.44
15	ATOM	738	O	HIS	398	22.121	2.887	40.730	1.00	44.91
	ATOM	739	N	PRO	399	20.755	4.049	42.096	1.00	46.45
	ATOM	740	CD	PRO	399	19.443	4.300	42.721	1.00	47.27
	ATOM	741	CA	PRO	399	21.785	4.968	42.586	1.00	45.35
	ATOM	742	CB	PRO	399	21.127	5.631	43.793	1.00	47.40
20	ATOM	743	CG	PRO	399	19.660	5.561	43.504	1.00	47.72
	ATOM	744	C	PRO	399	23.086	4.270	42.958	1.00	44.70
	ATOM	745	O	PRO	399	23.078	3.233	43.627	1.00	46.46
	ATOM	746	N	GLY	400	24.202	4.840	42.509	1.00	41.57
	ATOM	747	CA	GLY	400	25.506	4.281	42.813	1.00	39.84
25	ATOM	748	C	GLY	400	25.907	3.047	42.022	1.00	37.85
	ATOM	749	O	GLY	400	27.027	2.560	42.176	1.00	40.48
	ATOM	750	N	LYS	401	25.012	2.537	41.180	1.00	36.39
	ATOM	751	CA	LYS	401	25.315	1.344	40.390	1.00	34.47
	ATOM	752	CB	LYS	401	24.562	0.130	40.947	1.00	36.12
30	ATOM	753	CG	LYS	401	24.633	-0.007	42.466	1.00	39.30
	ATOM	754	CD	LYS	401	24.288	-1.429	42.903	1.00	44.38
	ATOM	755	CE	LYS	401	24.459	-1.605	44.408	1.00	46.68
	ATOM	756	NZ	LYS	401	24.968	-2.969	44.747	1.00	53.37
	ATOM	757	C	LYS	401	24.969	1.485	38.911	1.00	32.34
35	ATOM	758	O	LYS	401	24.141	2.308	38.531	1.00	31.16
	ATOM	759	N	LEU	402	25.612	0.663	38.086	1.00	28.52
	ATOM	760	CA	LEU	402	25.358	0.658	36.648	1.00	29.06
	ATOM	761	CB	LEU	402	26.661	0.847	35.867	1.00	29.26
	ATOM	762	CG	LEU	402	27.278	2.242	36.029	1.00	24.67
40	ATOM	763	CD1	LEU	402	28.623	2.310	35.310	1.00	27.47
	ATOM	764	CD2	LEU	402	26.312	3.277	35.482	1.00	24.93
	ATOM	765	C	LEU	402	24.755	-0.686	36.292	1.00	30.43
	ATOM	766	O	LEU	402	25.367	-1.727	36.535	1.00	31.36
	ATOM	767	N	LEU	403	23.552	-0.658	35.735	1.00	31.07
45	ATOM	768	CA	LEU	403	22.873	-1.880	35.335	1.00	32.96
	ATOM	769	CB	LEU	403	21.361	-1.693	35.434	1.00	33.86
	ATOM	770	CG	LEU	403	20.551	-2.991	35.415	1.00	39.29
	ATOM	771	CD1	LEU	403	20.584	-3.637	36.806	1.00	43.62
	ATOM	772	CD2	LEU	403	19.128	-2.689	34.998	1.00	41.32
50	ATOM	773	C	LEU	403	23.255	-2.218	33.899	1.00	30.06
	ATOM	774	O	LEU	403	22.543	-1.870	32.956	1.00	31.63
	ATOM	775	N	PHE	404	24.383	-2.893	33.733	1.00	29.19
	ATOM	776	CA	PHE	404	24.834	-3.256	32.403	1.00	28.93
	ATOM	777	CB	PHE	404	26.201	-3.929	32.493	1.00	30.05
55	ATOM	778	CG	PHE	404	27.305	-2.998	32.926	1.00	30.78
	ATOM	779	CD1	PHE	404	27.794	-3.033	34.228	1.00	32.91
	ATOM	780	CD2	PHE	404	27.848	-2.078	32.030	1.00	32.75
	ATOM	781	CE1	PHE	404	28.816	-2.160	34.638	1.00	34.73
	ATOM	782	CE2	PHE	404	28.864	-1.205	32.423	1.00	30.68
60	ATOM	783	CZ	PHE	404	29.350	-1.242	33.727	1.00	31.43
	ATOM	784	C	PHE	404	23.809	-4.181	31.756	1.00	30.80

5	ATOM	785	O	PHE	404	23.625	-4.175	30.538	1.00	28.09
	ATOM	786	N	ALA	405	23.138	-4.967	32.594	1.00	30.25
	ATOM	787	CA	ALA	405	22.104	-5.910	32.163	1.00	29.78
	ATOM	788	CB	ALA	405	22.745	-7.172	31.598	1.00	29.97
	ATOM	789	C	ALA	405	21.309	-6.237	33.429	1.00	31.95
10	ATOM	790	O	ALA	405	21.785	-5.995	34.535	1.00	32.36
	ATOM	791	N	PRO	406	20.088	-6.779	33.288	1.00	34.40
	ATOM	792	CD	PRO	406	19.356	-7.102	32.053	1.00	35.81
	ATOM	793	CA	PRO	406	19.303	-7.101	34.490	1.00	36.41
	ATOM	794	CB	PRO	406	17.985	-7.654	33.935	1.00	35.38
15	ATOM	795	CG	PRO	406	17.922	-7.153	32.519	1.00	36.49
	ATOM	796	C	PRO	406	19.997	-8.084	35.433	1.00	37.32
	ATOM	797	O	PRO	406	19.698	-8.112	36.626	1.00	38.34
	ATOM	798	N	ASN	407	20.924	-8.877	34.902	1.00	36.69
	ATOM	799	CA	ASN	407	21.652	-9.847	35.712	1.00	38.85
20	ATOM	800	CB	ASN	407	21.582	-11.243	35.083	1.00	39.69
	ATOM	801	CG	ASN	407	22.232	-11.306	33.711	1.00	44.10
	ATOM	802	OD1	ASN	407	22.345	-10.296	33.009	1.00	37.78
	ATOM	803	ND2	ASN	407	22.660	-12.503	33.319	1.00	45.74
	ATOM	804	C	ASN	407	23.100	-9.435	35.874	1.00	38.12
25	ATOM	805	O	ASN	407	23.965	-10.256	36.178	1.00	39.81
	ATOM	806	N	LEU	408	23.364	-8.149	35.671	1.00	37.80
	ATOM	807	CA	LEU	408	24.713	-7.631	35.799	1.00	36.89
	ATOM	808	CB	LEU	408	25.449	-7.720	34.459	1.00	36.09
	ATOM	809	CG	LEU	408	26.972	-7.609	34.550	1.00	35.08
30	ATOM	810	CD1	LEU	408	27.525	-8.775	35.354	1.00	39.15
	ATOM	811	CD2	LEU	408	27.578	-7.587	33.158	1.00	36.85
	ATOM	812	C	LEU	408	24.670	-6.187	36.286	1.00	40.55
	ATOM	813	O	LEU	408	24.646	-5.248	35.491	1.00	38.29
	ATOM	814	N	LEU	409	24.644	-6.034	37.607	1.00	39.50
35	ATOM	815	CA	LEU	409	24.606	-4.733	38.257	1.00	41.00
	ATOM	816	CB	LEU	409	23.392	-4.658	39.184	1.00	43.69
	ATOM	817	CG	LEU	409	23.164	-3.382	39.993	1.00	47.35
	ATOM	818	CD1	LEU	409	22.848	-2.233	39.058	1.00	47.09
	ATOM	819	CD2	LEU	409	22.014	-3.603	40.976	1.00	49.38
40	ATOM	820	C	LEU	409	25.894	-4.566	39.060	1.00	41.80
	ATOM	821	O	LEU	409	26.178	-5.358	39.960	1.00	41.00
	ATOM	822	N	LEU	410	26.676	-3.544	38.727	1.00	39.23
	ATOM	823	CA	LEU	410	27.931	-3.296	39.423	1.00	40.45
	ATOM	824	CB	LEU	410	29.106	-3.354	38.442	1.00	41.59
45	ATOM	825	CG	LEU	410	29.457	-4.660	37.716	1.00	44.87
	ATOM	826	CD1	LEU	410	30.972	-4.728	37.554	1.00	45.41
	ATOM	827	CD2	LEU	410	28.949	-5.872	38.484	1.00	47.02
	ATOM	828	C	LEU	410	27.946	-1.944	40.132	1.00	40.67
	ATOM	829	O	LEU	410	27.361	-0.970	39.652	1.00	40.22
50	ATOM	830	N	ASP	411	28.610	-1.890	41.281	1.00	41.57
	ATOM	831	CA	ASP	411	28.717	-0.640	42.025	1.00	42.69
	ATOM	832	CB	ASP	411	28.490	-0.874	43.528	1.00	44.44
	ATOM	833	CG	ASP	411	29.655	-1.578	44.210	1.00	46.70
	ATOM	834	OD1	ASP	411	29.537	-1.849	45.426	1.00	51.44
55	ATOM	835	OD2	ASP	411	30.680	-1.861	43.553	1.00	48.79
	ATOM	836	C	ASP	411	30.088	-0.016	41.779	1.00	43.70
	ATOM	837	O	ASP	411	30.933	-0.610	41.107	1.00	38.48
	ATOM	838	N	ARG	412	30.295	1.181	42.321	1.00	46.78
	ATOM	839	CA	ARG	412	31.554	1.905	42.171	1.00	49.97
60	ATOM	840	CB	ARG	412	31.601	3.090	43.138	1.00	51.28
	ATOM	841	CG	ARG	412	30.971	4.364	42.614	1.00	54.77

5	ATOM	842	CD	ARG	412	31.644	5.580	43.219	1.00	54.61
	ATOM	843	NE	ARG	412	33.071	5.615	42.912	1.00	56.53
	ATOM	844	CZ	ARG	412	33.827	6.708	42.985	1.00	61.90
	ATOM	845	NH1	ARG	412	33.291	7.866	43.356	1.00	63.48
	ATOM	846	NH2	ARG	412	35.120	6.645	42.682	1.00	61.21
10	ATOM	847	C	ARG	412	32.771	1.026	42.429	1.00	50.29
	ATOM	848	O	ARG	412	33.628	0.866	41.561	1.00	51.02
	ATOM	849	N	ASN	413	32.844	0.469	43.633	1.00	51.94
	ATOM	850	CA	ASN	413	33.969	-0.375	44.021	1.00	53.15
	ATOM	851	CB	ASN	413	33.719	-0.980	45.403	1.00	55.88
15	ATOM	852	CG	ASN	413	33.654	0.073	46.496	1.00	57.99
	ATOM	853	OD1	ASN	413	33.697	1.276	46.223	1.00	58.27
	ATOM	854	ND2	ASN	413	33.551	-0.375	47.742	1.00	57.90
	ATOM	855	C	ASN	413	34.235	-1.480	43.013	1.00	53.95
	ATOM	856	O	ASN	413	35.386	-1.743	42.659	1.00	53.67
20	ATOM	857	N	GLN	414	33.173	-2.129	42.547	1.00	55.33
	ATOM	858	CA	GLN	414	33.326	-3.198	41.573	1.00	55.42
	ATOM	859	CB	GLN	414	31.991	-3.904	41.343	1.00	55.44
	ATOM	860	CG	GLN	414	31.645	-4.933	42.391	1.00	56.07
	ATOM	861	CD	GLN	414	30.203	-5.376	42.336	1.00	57.40
25	ATOM	862	OE1	GLN	414	29.296	-4.536	42.402	1.00	60.22
	ATOM	863	NE2	GLN	414	29.973	-6.664	42.199	1.00	57.27
	ATOM	864	C	GLN	414	33.850	-2.630	40.259	1.00	55.51
	ATOM	865	O	GLN	414	34.654	-3.265	39.578	1.00	56.16
	ATOM	866	N	GLY	415	33.398	-1.430	39.910	1.00	57.07
30	ATOM	867	CA	GLY	415	33.849	-0.806	38.680	1.00	58.51
	ATOM	868	C	GLY	415	35.350	-0.582	38.689	1.00	61.10
	ATOM	869	O	GLY	415	36.023	-0.748	37.671	1.00	59.47
	ATOM	870	N	LYS	416	35.877	-0.211	39.851	1.00	62.77
	ATOM	871	CA	LYS	416	37.305	0.041	40.011	1.00	65.49
35	ATOM	872	CB	LYS	416	37.634	0.262	41.491	1.00	66.04
	ATOM	873	CG	LYS	416	38.121	1.663	41.823	1.00	68.71
	ATOM	874	CD	LYS	416	37.078	2.439	42.613	1.00	70.98
	ATOM	875	CE	LYS	416	37.404	2.448	44.100	1.00	71.84
	ATOM	876	NZ	LYS	416	36.225	2.079	44.933	1.00	71.95
40	ATOM	877	C	LYS	416	38.159	-1.105	39.472	1.00	66.41
	ATOM	878	O	LYS	416	39.361	-0.946	39.269	1.00	67.15
	ATOM	879	N	CYS	417	37.538	-2.257	39.238	1.00	67.33
	ATOM	880	CA	CYS	417	38.270	-3.414	38.741	1.00	68.16
	ATOM	881	CB	CYS	417	37.951	-4.642	39.602	1.00	70.88
45	ATOM	882	SG	CYS	417	38.592	-4.549	41.301	1.00	76.09
	ATOM	883	C	CYS	417	38.015	-3.736	37.270	1.00	67.54
	ATOM	884	O	CYS	417	38.632	-4.653	36.720	1.00	68.48
	ATOM	885	N	VAL	418	37.111	-2.994	36.631	1.00	64.67
	ATOM	886	CA	VAL	418	36.817	-3.226	35.218	1.00	59.97
50	ATOM	887	CB	VAL	418	35.326	-2.917	34.879	1.00	59.60
	ATOM	888	CG1	VAL	418	34.971	-1.503	35.284	1.00	59.13
	ATOM	889	CG2	VAL	418	35.072	-3.121	33.391	1.00	54.85
	ATOM	890	C	VAL	418	37.739	-2.362	34.355	1.00	58.37
	ATOM	891	O	VAL	418	37.799	-1.140	34.512	1.00	55.44
55	ATOM	892	N	GLU	419	38.463	-3.012	33.450	1.00	56.02
	ATOM	893	CA	GLU	419	39.403	-2.328	32.570	1.00	54.28
	ATOM	894	CB	GLU	419	40.149	-3.351	31.710	1.00	57.57
	ATOM	895	CG	GLU	419	39.385	-3.779	30.468	1.00	60.87
	ATOM	896	CD	GLU	419	40.179	-4.722	29.584	1.00	63.34
60	ATOM	897	OE1	GLU	419	40.432	-5.870	30.011	1.00	64.90
	ATOM	898	OE2	GLU	419	40.546	-4.313	28.462	1.00	63.18

5	ATOM	899	C	GLU	419	38.761	-1.281	31.662	1.00	52.05
	ATOM	900	O	GLU	419	37.665	-1.481	31.131	1.00	49.82
	ATOM	901	N	GLY	420	39.465	-0.165	31.491	1.00	49.45
	ATOM	902	CA	GLY	420	38.983	0.908	30.642	1.00	46.22
	ATOM	903	C	GLY	420	37.895	1.767	31.254	1.00	44.55
10	ATOM	904	O	GLY	420	37.417	2.705	30.619	1.00	42.08
	ATOM	905	N	MET	421	37.503	1.471	32.488	1.00	43.41
	ATOM	906	CA	MET	421	36.449	2.248	33.123	1.00	42.48
	ATOM	907	CB	MET	421	35.306	1.327	33.554	1.00	42.34
	ATOM	908	CG	MET	421	34.590	0.635	32.396	1.00	38.22
15	ATOM	909	SD	MET	421	32.927	0.102	32.843	1.00	38.56
	ATOM	910	CE	MET	421	32.003	1.699	32.766	1.00	35.54
	ATOM	911	C	MET	421	36.923	3.059	34.312	1.00	41.64
	ATOM	912	O	MET	421	36.113	3.512	35.111	1.00	39.77
	ATOM	913	N	VAL	422	38.232	3.256	34.430	1.00	43.42
20	ATOM	914	CA	VAL	422	38.757	4.019	35.557	1.00	44.79
	ATOM	915	CB	VAL	422	40.285	4.248	35.433	1.00	46.54
	ATOM	916	CG1	VAL	422	40.595	5.086	34.206	1.00	48.25
	ATOM	917	CG2	VAL	422	40.813	4.920	36.696	1.00	46.24
	ATOM	918	C	VAL	422	38.056	5.372	35.689	1.00	44.09
25	ATOM	919	O	VAL	422	37.691	5.783	36.783	1.00	44.12
	ATOM	920	N	GLU	423	37.846	6.055	34.570	1.00	42.07
	ATOM	921	CA	GLU	423	37.192	7.356	34.616	1.00	40.24
	ATOM	922	CB	GLU	423	37.909	8.338	33.684	1.00	44.02
	ATOM	923	CG	GLU	423	39.411	8.467	33.893	1.00	50.04
30	ATOM	924	CD	GLU	423	40.096	9.158	32.719	1.00	55.64
	ATOM	925	OE1	GLU	423	39.539	10.156	32.205	1.00	56.66
	ATOM	926	OE2	GLU	423	41.188	8.703	32.306	1.00	58.02
	ATOM	927	C	GLU	423	35.704	7.337	34.250	1.00	35.77
	ATOM	928	O	GLU	423	34.881	7.955	34.919	1.00	33.20
35	ATOM	929	N	ILE	424	35.345	6.617	33.197	1.00	36.16
	ATOM	930	CA	ILE	424	33.949	6.643	32.771	1.00	31.63
	ATOM	931	CB	ILE	424	33.803	6.087	31.347	1.00	33.58
	ATOM	932	CG2	ILE	424	34.639	6.936	30.395	1.00	33.48
	ATOM	933	CG1	ILE	424	34.204	4.617	31.296	1.00	34.46
40	ATOM	934	CD1	ILE	424	33.857	3.955	29.978	1.00	34.67
	ATOM	935	C	ILE	424	32.890	6.035	33.685	1.00	28.89
	ATOM	936	O	ILE	424	31.729	6.443	33.632	1.00	26.49
	ATOM	937	N	PHE	425	33.261	5.091	34.542	1.00	29.26
	ATOM	938	CA	PHE	425	32.257	4.520	35.447	1.00	29.87
45	ATOM	939	CB	PHE	425	32.903	3.529	36.423	1.00	31.26
	ATOM	940	CG	PHE	425	31.948	2.496	36.959	1.00	32.17
	ATOM	941	CD1	PHE	425	31.124	2.783	38.048	1.00	33.70
	ATOM	942	CD2	PHE	425	31.881	1.230	36.381	1.00	30.64
	ATOM	943	CE1	PHE	425	30.244	1.814	38.563	1.00	32.60
50	ATOM	944	CE2	PHE	425	31.010	0.256	36.881	1.00	31.55
	ATOM	945	CZ	PHE	425	30.189	0.549	37.973	1.00	33.34
	ATOM	946	C	PHE	425	31.594	5.649	36.240	1.00	30.17
	ATOM	947	O	PHE	425	30.368	5.774	36.276	1.00	26.71
	ATOM	948	N	ASP	426	32.415	6.483	36.870	1.00	29.45
55	ATOM	949	CA	ASP	426	31.893	7.587	37.661	1.00	32.29
	ATOM	950	CB	ASP	426	33.031	8.291	38.401	1.00	33.49
	ATOM	951	CG	ASP	426	33.455	7.546	39.655	1.00	39.42
	ATOM	952	OD1	ASP	426	32.767	6.574	40.038	1.00	38.35
	ATOM	953	OD2	ASP	426	34.480	7.934	40.256	1.00	39.58
60	ATOM	954	C	ASP	426	31.133	8.592	36.806	1.00	29.02
	ATOM	955	O	ASP	426	30.154	9.175	37.257	1.00	31.34

5	ATOM	956	N	MET	427	31.585	8.797	35.572	1.00	30.69
	ATOM	957	CA	MET	427	30.919	9.736	34.675	1.00	28.63
	ATOM	958	CB	MET	427	31.744	9.912	33.407	1.00	26.83
	ATOM	959	CG	MET	427	33.032	10.680	33.608	1.00	31.41
	ATOM	960	SD	MET	427	33.962	10.783	32.077	1.00	34.87
10	ATOM	961	CE	MET	427	35.409	11.753	32.643	1.00	44.60
	ATOM	962	C	MET	427	29.526	9.202	34.324	1.00	28.70
	ATOM	963	O	MET	427	28.536	9.947	34.302	1.00	25.01
	ATOM	964	N	LEU	428	29.451	7.902	34.057	1.00	25.13
	ATOM	965	CA	LEU	428	28.173	7.292	33.730	1.00	27.60
15	ATOM	966	CB	LEU	428	28.379	5.824	33.332	1.00	28.00
	ATOM	967	CG	LEU	428	29.039	5.682	31.957	1.00	26.99
	ATOM	968	CD1	LEU	428	29.678	4.303	31.782	1.00	27.80
	ATOM	969	CD2	LEU	428	27.995	5.927	30.894	1.00	25.33
	ATOM	970	C	LEU	428	27.210	7.412	34.916	1.00	29.59
20	ATOM	971	O	LEU	428	26.041	7.743	34.743	1.00	27.07
	ATOM	972	N	LEU	429	27.701	7.147	36.126	1.00	30.40
	ATOM	973	CA	LEU	429	26.859	7.251	37.323	1.00	30.59
	ATOM	974	CB	LEU	429	27.675	6.884	38.571	1.00	31.76
	ATOM	975	CG	LEU	429	28.078	5.415	38.757	1.00	32.43
25	ATOM	976	CD1	LEU	429	28.961	5.264	39.995	1.00	31.60
	ATOM	977	CD2	LEU	429	26.825	4.573	38.903	1.00	34.66
	ATOM	978	C	LEU	429	26.319	8.681	37.466	1.00	30.46
	ATOM	979	O	LEU	429	25.143	8.901	37.769	1.00	28.40
	ATOM	980	N	ALA	430	27.193	9.656	37.237	1.00	31.34
30	ATOM	981	CA	ALA	430	26.806	11.059	37.332	1.00	29.83
	ATOM	982	CB	ALA	430	28.017	11.951	37.078	1.00	31.29
	ATOM	983	C	ALA	430	25.696	11.387	36.344	1.00	31.04
	ATOM	984	O	ALA	430	24.753	12.107	36.674	1.00	30.79
	ATOM	985	N	THR	431	25.802	10.854	35.128	1.00	30.30
35	ATOM	986	CA	THR	431	24.786	11.105	34.112	1.00	28.81
	ATOM	987	CB	THR	431	25.207	10.533	32.737	1.00	30.55
	ATOM	988	OG1	THR	431	26.569	10.893	32.465	1.00	31.88
	ATOM	989	CG2	THR	431	24.321	11.087	31.634	1.00	25.63
	ATOM	990	C	THR	431	23.462	10.481	34.530	1.00	29.49
40	ATOM	991	O	THR	431	22.402	11.099	34.397	1.00	26.18
	ATOM	992	N	SER	432	23.520	9.253	35.037	1.00	28.11
	ATOM	993	CA	SER	432	22.308	8.573	35.480	1.00	29.78
	ATOM	994	CB	SER	432	22.639	7.177	36.008	1.00	33.11
	ATOM	995	OG	SER	432	21.454	6.412	36.136	1.00	36.92
45	ATOM	996	C	SER	432	21.651	9.399	36.589	1.00	31.49
	ATOM	997	O	SER	432	20.433	9.576	36.613	1.00	30.09
	ATOM	998	N	ASER	433	22.476	9.901	37.496	0.75	32.09
	ATOM	999	N	BSER	433	22.474	9.906	37.500	0.25	31.10
	ATOM	1000	CA	ASER	433	22.002	10.715	38.605	0.75	35.68
50	ATOM	1001	CA	BSER	433	21.985	10.717	38.608	0.25	32.21
	ATOM	1002	CB	ASER	433	23.185	11.097	39.502	0.75	37.18
	ATOM	1003	CB	BSER	433	23.145	11.104	39.529	0.25	31.45
	ATOM	1004	OG	ASER	433	22.823	12.090	40.443	0.75	44.09
	ATOM	1005	OG	BSER	433	23.785	9.953	40.053	0.25	29.52
55	ATOM	1006	C	ASER	433	21.299	11.971	38.091	0.75	35.01
	ATOM	1007	C	BSER	433	21.295	11.976	38.092	0.25	32.88
	ATOM	1008	O	ASER	433	20.257	12.373	38.612	0.75	35.34
	ATOM	1009	O	BSER	433	20.264	12.391	38.622	0.25	33.42
	ATOM	1010	N	ARG	434	21.867	12.579	37.054	1.00	33.38
60	ATOM	1011	CA	ARG	434	21.300	13.788	36.470	1.00	34.19
	ATOM	1012	CB	ARG	434	22.239	14.354	35.400	1.00	33.89

5	ATOM	1013	CG	ARG	434	21.670	15.528	34.625	1.00	38.30
	ATOM	1014	CD	ARG	434	21.559	16.787	35.479	1.00	37.91
	ATOM	1015	NE	ARG	434	21.158	17.944	34.680	1.00	37.78
	ATOM	1016	CZ	ARG	434	20.488	18.995	35.149	1.00	41.06
	ATOM	1017	NH1	ARG	434	20.132	19.049	36.428	1.00	40.70
10	ATOM	1018	NH2	ARG	434	20.175	19.998	34.337	1.00	38.78
	ATOM	1019	C	ARG	434	19.937	13.491	35.873	1.00	33.48
	ATOM	1020	O	ARG	434	18.996	14.266	36.053	1.00	30.54
	ATOM	1021	N	PHE	435	19.831	12.371	35.158	1.00	34.68
	ATOM	1022	CA	PHE	435	18.563	11.963	34.549	1.00	35.02
15	ATOM	1023	CB	PHE	435	18.727	10.634	33.796	1.00	34.96
	ATOM	1024	CG	PHE	435	19.240	10.779	32.386	1.00	37.63
	ATOM	1025	CD1	PHE	435	19.459	12.035	31.824	1.00	42.03
	ATOM	1026	CD2	PHE	435	19.521	9.649	31.623	1.00	41.24
	ATOM	1027	CE1	PHE	435	19.953	12.164	30.521	1.00	43.11
20	ATOM	1028	CE2	PHE	435	20.016	9.768	30.322	1.00	40.59
	ATOM	1029	CZ	PHE	435	20.233	11.029	29.775	1.00	40.63
	ATOM	1030	C	PHE	435	17.527	11.780	35.657	1.00	35.49
	ATOM	1031	O	PHE	435	16.361	12.135	35.496	1.00	34.78
	ATOM	1032	N	ARG	436	17.968	11.216	36.777	1.00	38.27
25	ATOM	1033	CA	ARG	436	17.094	10.982	37.924	1.00	40.67
	ATOM	1034	CB	ARG	436	17.844	10.215	39.012	1.00	40.70
	ATOM	1035	CG	ARG	436	16.942	9.590	40.068	1.00	44.98
	ATOM	1036	CD	ARG	436	17.648	8.459	40.810	1.00	48.09
	ATOM	1037	NE	ARG	436	18.982	8.841	41.275	1.00	50.16
30	ATOM	1038	CZ	ARG	436	20.119	8.361	40.777	1.00	52.19
	ATOM	1039	NH1	ARG	436	20.099	7.472	39.790	1.00	49.34
	ATOM	1040	NH2	ARG	436	21.283	8.770	41.266	1.00	51.85
	ATOM	1041	C	ARG	436	16.576	12.302	38.493	1.00	40.40
	ATOM	1042	O	ARG	436	15.382	12.458	38.730	1.00	41.49
35	ATOM	1043	N	MET	437	17.477	13.252	38.706	1.00	40.02
	ATOM	1044	CA	MET	437	17.090	14.546	39.245	1.00	41.02
	ATOM	1045	CB	MET	437	18.329	15.427	39.440	1.00	40.29
	ATOM	1046	C	MET	437	16.099	15.221	38.299	1.00	40.81
	ATOM	1047	O	MET	437	15.111	15.805	38.734	1.00	42.46
40	ATOM	1048	N	MET	438	16.367	15.127	37.001	1.00	39.02
	ATOM	1049	CA	MET	438	15.510	15.732	35.988	1.00	40.11
	ATOM	1050	CB	MET	438	16.237	15.793	34.651	1.00	38.16
	ATOM	1051	CG	MET	438	17.352	16.794	34.601	1.00	41.52
	ATOM	1052	SD	MET	438	17.999	16.862	32.943	1.00	43.94
45	ATOM	1053	CE	MET	438	16.698	17.748	32.096	1.00	39.96
	ATOM	1054	C	MET	438	14.221	14.964	35.783	1.00	37.72
	ATOM	1055	O	MET	438	13.305	15.451	35.125	1.00	36.82
	ATOM	1056	N	ASN	439	14.155	13.759	36.337	1.00	38.81
	ATOM	1057	CA	ASN	439	12.981	12.919	36.174	1.00	40.77
50	ATOM	1058	CB	ASN	439	11.762	13.556	36.847	1.00	44.52
	ATOM	1059	CG	ASN	439	10.566	12.620	36.887	1.00	48.29
	ATOM	1060	OD1	ASN	439	10.721	11.400	36.964	1.00	48.48
	ATOM	1061	ND2	ASN	439	9.365	13.189	36.829	1.00	50.23
	ATOM	1062	C	ASN	439	12.725	12.744	34.677	1.00	39.36
55	ATOM	1063	O	ASN	439	11.637	13.037	34.172	1.00	37.76
	ATOM	1064	N	LEU	440	13.749	12.274	33.972	1.00	37.65
	ATOM	1065	CA	LEU	440	13.655	12.052	32.532	1.00	35.22
	ATOM	1066	CB	LEU	440	14.999	11.576	31.987	1.00	34.70
	ATOM	1067	CG	LEU	440	15.022	11.467	30.462	1.00	35.45
60	ATOM	1068	CD1	LEU	440	14.890	12.862	29.869	1.00	35.24
	ATOM	1069	CD2	LEU	440	16.297	10.795	29.999	1.00	35.30

5	ATOM	1070	C	LEU	440	12.587	11.024	32.196	1.00	36.48
	ATOM	1071	O	LEU	440	12.518	9.967	32.826	1.00	37.36
	ATOM	1072	N	GLN	441	11.763	11.328	31.197	1.00	36.82
	ATOM	1073	CA	GLN	441	10.696	10.420	30.785	1.00	38.51
	ATOM	1074	CB	GLN	441	9.431	11.211	30.443	1.00	38.23
10	ATOM	1075	CG	GLN	441	8.912	12.063	31.592	1.00	42.46
	ATOM	1076	CD	GLN	441	8.362	11.227	32.729	1.00	44.91
	ATOM	1077	OE1	GLN	441	7.268	10.668	32.629	1.00	47.31
	ATOM	1078	NE2	GLN	441	9.119	11.132	33.818	1.00	44.06
	ATOM	1079	C	GLN	441	11.099	9.565	29.585	1.00	38.48
15	ATOM	1080	O	GLN	441	11.923	9.976	28.763	1.00	35.80
	ATOM	1081	N	GLY	442	10.500	8.378	29.494	1.00	36.03
	ATOM	1082	CA	GLY	442	10.792	7.468	28.401	1.00	37.72
	ATOM	1083	C	GLY	442	10.599	8.112	27.043	1.00	36.88
	ATOM	1084	O	GLY	442	11.381	7.877	26.123	1.00	33.72
20	ATOM	1085	N	GLU	443	9.556	8.925	26.918	1.00	36.59
	ATOM	1086	CA	GLU	443	9.269	9.603	25.661	1.00	37.13
	ATOM	1087	CB	GLU	443	7.956	10.379	25.764	1.00	41.57
	ATOM	1088	CG	GLU	443	6.723	9.488	25.879	1.00	47.76
	ATOM	1089	CD	GLU	443	6.483	9.008	27.302	1.00	53.96
25	ATOM	1090	OE1	GLU	443	5.619	8.123	27.498	1.00	57.66
	ATOM	1091	OE2	GLU	443	7.159	9.515	28.225	1.00	56.13
	ATOM	1092	C	GLU	443	10.408	10.551	25.311	1.00	35.27
	ATOM	1093	O	GLU	443	10.759	10.704	24.145	1.00	33.85
	ATOM	1094	N	GLU	444	10.984	11.179	26.331	1.00	32.09
30	ATOM	1095	CA	GLU	444	12.097	12.095	26.126	1.00	33.92
	ATOM	1096	CB	GLU	444	12.332	12.924	27.388	1.00	34.97
	ATOM	1097	CG	GLU	444	11.169	13.845	27.732	1.00	38.28
	ATOM	1098	CD	GLU	444	11.383	14.610	29.023	1.00	38.11
	ATOM	1099	OE1	GLU	444	11.800	13.993	30.026	1.00	39.53
35	ATOM	1100	OE2	GLU	444	11.132	15.834	29.036	1.00	40.77
	ATOM	1101	C	GLU	444	13.356	11.305	25.770	1.00	33.59
	ATOM	1102	O	GLU	444	14.085	11.670	24.842	1.00	33.35
	ATOM	1103	N	PHE	445	13.590	10.215	26.501	1.00	30.68
	ATOM	1104	CA	PHE	445	14.753	9.357	26.276	1.00	32.49
40	ATOM	1105	CB	PHE	445	14.703	8.139	27.203	1.00	29.35
	ATOM	1106	CG	PHE	445	15.667	7.047	26.828	1.00	30.78
	ATOM	1107	CD1	PHE	445	17.036	7.201	27.030	1.00	28.25
	ATOM	1108	CD2	PHE	445	15.205	5.863	26.266	1.00	30.62
	ATOM	1109	CE1	PHE	445	17.933	6.195	26.675	1.00	28.67
45	ATOM	1110	CE2	PHE	445	16.095	4.848	25.908	1.00	31.37
	ATOM	1111	CZ	PHE	445	17.460	5.015	26.113	1.00	30.37
	ATOM	1112	C	PHE	445	14.850	8.885	24.829	1.00	31.11
	ATOM	1113	O	PHE	445	15.924	8.947	24.221	1.00	32.20
	ATOM	1114	N	VAL	446	13.739	8.415	24.266	1.00	28.63
50	ATOM	1115	CA	VAL	446	13.787	7.943	22.889	1.00	27.94
	ATOM	1116	CB	VAL	446	12.478	7.193	22.478	1.00	28.48
	ATOM	1117	CG1	VAL	446	12.318	5.939	23.343	1.00	29.61
	ATOM	1118	CG2	VAL	446	11.265	8.092	22.607	1.00	27.23
	ATOM	1119	C	VAL	446	14.099	9.064	21.900	1.00	27.28
55	ATOM	1120	O	VAL	446	14.781	8.837	20.904	1.00	28.07
	ATOM	1121	N	CYS	447	13.619	10.275	22.166	1.00	28.97
	ATOM	1122	CA	CYS	447	13.919	11.394	21.272	1.00	29.14
	ATOM	1123	CB	CYS	447	13.156	12.653	21.693	1.00	28.90
	ATOM	1124	SG	CYS	447	11.389	12.591	21.309	1.00	35.68
60	ATOM	1125	C	CYS	447	15.420	11.677	21.328	1.00	28.03
	ATOM	1126	O	CYS	447	16.063	11.885	20.302	1.00	29.34



5	ATOM	1127	N	LEU	448	15.969	11.686	22.538	1.00	27.28
	ATOM	1128	CA	LEU	448	17.392	11.938	22.729	1.00	25.30
	ATOM	1129	CB	LEU	448	17.733	11.932	24.220	1.00	27.72
	ATOM	1130	CG	LEU	448	17.248	13.135	25.040	1.00	29.54
	ATOM	1131	CD1	LEU	448	17.807	13.042	26.454	1.00	30.85
10	ATOM	1132	CD2	LEU	448	17.688	14.434	24.376	1.00	30.24
	ATOM	1133	C	LEU	448	18.245	10.902	22.008	1.00	27.62
	ATOM	1134	O	LEU	448	19.207	11.252	21.327	1.00	25.10
	ATOM	1135	N	LYS	449	17.905	9.621	22.162	1.00	25.16
	ATOM	1136	CA	LYS	449	18.673	8.570	21.506	1.00	27.55
15	ATOM	1137	CB	LYS	449	18.135	7.185	21.900	1.00	28.99
	ATOM	1138	CG	LYS	449	19.134	6.052	21.694	1.00	34.70
	ATOM	1139	CD	LYS	449	18.737	4.789	22.459	1.00	32.67
	ATOM	1140	CE	LYS	449	17.267	4.419	22.220	1.00	31.87
	ATOM	1141	NZ	LYS	449	17.022	2.967	22.472	1.00	29.14
20	ATOM	1142	C	LYS	449	18.626	8.749	19.990	1.00	25.88
	ATOM	1143	O	LYS	449	19.610	8.489	19.296	1.00	25.93
	ATOM	1144	N	SER	450	17.482	9.197	19.480	1.00	26.07
	ATOM	1145	CA	SER	450	17.323	9.421	18.052	1.00	27.24
	ATOM	1146	CB	SER	450	15.857	9.705	17.721	1.00	32.24
25	ATOM	1147	OG	SER	450	15.098	8.519	17.779	1.00	34.94
	ATOM	1148	C	SER	450	18.176	10.607	17.618	1.00	26.78
	ATOM	1149	O	SER	450	18.763	10.598	16.535	1.00	25.85
	ATOM	1150	N	ILE	451	18.231	11.632	18.463	1.00	26.94
	ATOM	1151	CA	ILE	451	19.032	12.810	18.155	1.00	26.13
30	ATOM	1152	CB	ILE	451	18.950	13.850	19.291	1.00	27.72
	ATOM	1153	CG2	ILE	451	20.019	14.929	19.101	1.00	20.53
	ATOM	1154	CG1	ILE	451	17.553	14.475	19.322	1.00	29.49
	ATOM	1155	CD1	ILE	451	17.377	15.473	20.447	1.00	36.24
	ATOM	1156	C	ILE	451	20.489	12.381	17.989	1.00	24.88
35	ATOM	1157	O	ILE	451	21.161	12.771	17.034	1.00	26.96
	ATOM	1158	N	ILE	452	20.977	11.582	18.931	1.00	22.72
	ATOM	1159	CA	ILE	452	22.359	11.120	18.880	1.00	21.95
	ATOM	1160	CB	ILE	452	22.660	10.155	20.050	1.00	23.57
	ATOM	1161	CG2	ILE	452	23.982	9.435	19.804	1.00	22.10
40	ATOM	1162	CG1	ILE	452	22.718	10.949	21.371	1.00	21.70
	ATOM	1163	CD1	ILE	452	22.768	10.060	22.624	1.00	25.30
	ATOM	1164	C	ILE	452	22.656	10.419	17.557	1.00	23.02
	ATOM	1165	O	ILE	452	23.650	10.708	16.885	1.00	21.25
	ATOM	1166	N	LEU	453	21.779	9.497	17.173	1.00	22.83
45	ATOM	1167	CA	LEU	453	21.984	8.768	15.935	1.00	22.05
	ATOM	1168	CB	LEU	453	20.843	7.764	15.733	1.00	22.06
	ATOM	1169	CG	LEU	453	20.712	7.189	14.324	1.00	22.03
	ATOM	1170	CD1	LEU	453	21.815	6.165	14.107	1.00	24.81
	ATOM	1171	CD2	LEU	453	19.328	6.535	14.156	1.00	24.73
50	ATOM	1172	C	LEU	453	22.092	9.687	14.717	1.00	23.95
	ATOM	1173	O	LEU	453	22.962	9.501	13.860	1.00	24.60
	ATOM	1174	N	LEU	454	21.220	10.687	14.638	1.00	26.72
	ATOM	1175	CA	LEU	454	21.234	11.599	13.494	1.00	26.45
	ATOM	1176	CB	LEU	454	19.852	12.242	13.330	1.00	25.51
55	ATOM	1177	CG	LEU	454	18.737	11.222	13.052	1.00	30.16
	ATOM	1178	CD1	LEU	454	17.405	11.926	12.955	1.00	28.76
	ATOM	1179	CD2	LEU	454	19.037	10.478	11.759	1.00	32.59
	ATOM	1180	C	LEU	454	22.292	12.703	13.552	1.00	28.24
	ATOM	1181	O	LEU	454	22.778	13.148	12.513	1.00	29.06
60	ATOM	1182	N	ASN	455	22.638	13.146	14.757	1.00	26.56
	ATOM	1183	CA	ASN	455	23.604	14.236	14.934	1.00	26.79

5	ATOM	1184	CB	ASN	455	23.284	14.998	16.224	1.00	26.20
	ATOM	1185	CG	ASN	455	24.174	16.217	16.419	1.00	27.26
	ATOM	1186	OD1	ASN	455	24.171	17.134	15.602	1.00	30.83
	ATOM	1187	ND2	ASN	455	24.931	16.230	17.506	1.00	27.16
	ATOM	1188	C	ASN	455	25.062	13.782	14.954	1.00	30.63
10	ATOM	1189	O	ASN	455	25.965	14.517	14.525	1.00	27.69
	ATOM	1190	N	SER	456	25.268	12.569	15.461	1.00	30.48
	ATOM	1191	CA	SER	456	26.572	11.928	15.579	1.00	35.26
	ATOM	1192	CB	SER	456	26.393	10.393	15.505	1.00	39.69
	ATOM	1193	OG	SER	456	25.871	9.953	14.243	1.00	30.73
15	ATOM	1194	C	SER	456	27.627	12.344	14.562	1.00	35.56
	ATOM	1195	O	SER	456	28.599	13.041	14.884	1.00	33.00
	ATOM	1196	N	GLY	457	27.437	11.886	13.334	1.00	33.88
	ATOM	1197	CA	GLY	457	28.393	12.189	12.292	1.00	36.77
	ATOM	1198	C	GLY	457	27.876	13.017	11.136	1.00	37.02
20	ATOM	1199	O	GLY	457	28.310	12.805	10.013	1.00	38.66
	ATOM	1200	N	VAL	458	26.967	13.956	11.392	1.00	39.12
	ATOM	1201	CA	VAL	458	26.438	14.802	10.317	1.00	43.81
	ATOM	1202	CB	VAL	458	25.231	15.648	10.755	1.00	44.25
	ATOM	1203	CG1	VAL	458	24.209	15.713	9.631	1.00	44.51
25	ATOM	1204	CG2	VAL	458	24.638	15.098	12.013	1.00	50.53
	ATOM	1205	C	VAL	458	27.472	15.801	9.817	1.00	46.72
	ATOM	1206	O	VAL	458	27.391	16.265	8.681	1.00	47.08
	ATOM	1207	N	TYR	459	28.432	16.144	10.670	1.00	50.74
	ATOM	1208	CA	TYR	459	29.456	17.114	10.301	1.00	55.43
30	ATOM	1209	CB	TYR	459	29.647	18.129	11.433	1.00	56.62
	ATOM	1210	CG	TYR	459	28.375	18.870	11.781	1.00	59.34
	ATOM	1211	CD1	TYR	459	28.094	19.229	13.095	1.00	60.73
	ATOM	1212	CE1	TYR	459	26.900	19.867	13.429	1.00	62.14
	ATOM	1213	CD2	TYR	459	27.430	19.175	10.795	1.00	62.16
35	ATOM	1214	CE2	TYR	459	26.234	19.812	11.118	1.00	63.83
	ATOM	1215	CZ	TYR	459	25.976	20.154	12.437	1.00	62.88
	ATOM	1216	OH	TYR	459	24.790	20.764	12.767	1.00	62.56
	ATOM	1217	C	TYR	459	30.791	16.489	9.928	1.00	57.21
	ATOM	1218	O	TYR	459	31.793	17.189	9.798	1.00	56.86
40	ATOM	1219	N	THR	460	30.800	15.173	9.750	1.00	59.22
	ATOM	1220	CA	THR	460	32.018	14.474	9.366	1.00	62.25
	ATOM	1221	CB	THR	460	32.502	13.531	10.499	1.00	63.07
	ATOM	1222	OG1	THR	460	33.474	12.613	9.983	1.00	67.80
	ATOM	1223	CG2	THR	460	31.344	12.759	11.084	1.00	60.23
45	ATOM	1224	C	THR	460	31.759	13.678	8.086	1.00	63.54
	ATOM	1225	O	THR	460	32.457	12.708	7.782	1.00	63.91
	ATOM	1226	N	PHE	461	30.758	14.113	7.326	1.00	65.06
	ATOM	1227	CA	PHE	461	30.395	13.446	6.080	1.00	67.00
	ATOM	1228	CB	PHE	461	29.052	13.975	5.563	1.00	66.48
50	ATOM	1229	CG	PHE	461	27.867	13.147	5.991	1.00	66.30
	ATOM	1230	CD1	PHE	461	26.657	13.754	6.312	1.00	65.58
	ATOM	1231	CD2	PHE	461	27.963	11.760	6.085	1.00	66.41
	ATOM	1232	CE1	PHE	461	25.562	12.996	6.723	1.00	65.45
	ATOM	1233	CE2	PHE	461	26.872	10.994	6.494	1.00	66.83
55	ATOM	1234	CZ	PHE	461	25.670	11.616	6.814	1.00	65.12
	ATOM	1235	C	PHE	461	31.463	13.604	5.004	1.00	68.38
	ATOM	1236	O	PHE	461	32.181	14.606	4.962	1.00	68.98
	ATOM	1237	N	LEU	462	31.542	12.601	4.132	1.00	69.57
	ATOM	1238	CA	LEU	462	32.511	12.545	3.039	1.00	71.68
60	ATOM	1239	CB	LEU	462	32.080	11.475	2.030	1.00	71.00
	ATOM	1240	C	LEU	462	32.810	13.856	2.304	1.00	72.40

5	ATOM	1241	O	LEU	462	33.725	14.590	2.680	1.00	73.45
	ATOM	1242	N	SER	463	32.043	14.141	1.253	1.00	73.22
	ATOM	1243	CA	SER	463	32.262	15.343	0.449	1.00	72.61
	ATOM	1244	CB	SER	463	32.544	14.942	-1.005	1.00	73.38
	ATOM	1245	C	SER	463	31.126	16.362	0.491	1.00	71.17
10	ATOM	1246	O	SER	463	30.455	16.528	1.511	1.00	72.05
	ATOM	1247	N	SER	464	30.932	17.049	-0.633	1.00	68.86
	ATOM	1248	CA	SER	464	29.892	18.063	-0.759	1.00	66.06
	ATOM	1249	CB	SER	464	30.514	19.457	-0.704	1.00	66.26
	ATOM	1250	C	SER	464	29.108	17.887	-2.060	1.00	63.72
15	ATOM	1251	O	SER	464	28.657	18.862	-2.662	1.00	62.88
	ATOM	1252	N	THR	465	28.954	16.638	-2.493	1.00	60.93
	ATOM	1253	CA	THR	465	28.205	16.343	-3.709	1.00	57.47
	ATOM	1254	CB	THR	465	28.185	14.824	-4.004	1.00	57.80
	ATOM	1255	OG1	THR	465	27.525	14.135	-2.934	1.00	54.75
20	ATOM	1256	CG2	THR	465	29.606	14.287	-4.149	1.00	57.49
	ATOM	1257	C	THR	465	26.767	16.824	-3.523	1.00	54.93
	ATOM	1258	O	THR	465	26.349	17.129	-2.407	1.00	54.26
	ATOM	1259	N	LEU	466	26.013	16.892	-4.614	1.00	51.85
	ATOM	1260	CA	LEU	466	24.625	17.330	-4.550	1.00	49.25
25	ATOM	1261	CB	LEU	466	24.013	17.349	-5.956	1.00	48.74
	ATOM	1262	CG	LEU	466	22.953	18.415	-6.253	1.00	48.72
	ATOM	1263	CD1	LEU	466	22.156	18.002	-7.482	1.00	48.32
	ATOM	1264	CD2	LEU	466	22.033	18.594	-5.057	1.00	48.14
	ATOM	1265	C	LEU	466	23.817	16.397	-3.650	1.00	48.16
30	ATOM	1266	O	LEU	466	22.961	16.845	-2.883	1.00	45.90
	ATOM	1267	N	LYS	467	24.093	15.099	-3.750	1.00	46.47
	ATOM	1268	CA	LYS	467	23.399	14.100	-2.947	1.00	47.45
	ATOM	1269	CB	LYS	467	23.802	12.693	-3.395	1.00	49.38
	ATOM	1270	CG	LYS	467	22.829	11.602	-2.974	1.00	52.70
35	ATOM	1271	CD	LYS	467	23.561	10.301	-2.682	1.00	56.48
	ATOM	1272	CE	LYS	467	23.105	9.180	-3.604	1.00	59.54
	ATOM	1273	NZ	LYS	467	24.150	8.117	-3.732	1.00	61.22
	ATOM	1274	C	LYS	467	23.738	14.284	-1.472	1.00	46.89
	ATOM	1275	O	LYS	467	22.884	14.108	-0.604	1.00	46.06
40	ATOM	1276	N	SER	468	24.989	14.644	-1.202	1.00	45.82
	ATOM	1277	CA	SER	468	25.457	14.854	0.160	1.00	46.82
	ATOM	1278	CB	SER	468	26.976	15.050	0.173	1.00	47.85
	ATOM	1279	OG	SER	468	27.407	15.537	1.435	1.00	55.73
	ATOM	1280	C	SER	468	24.778	16.063	0.790	1.00	44.24
45	ATOM	1281	O	SER	468	24.473	16.062	1.983	1.00	42.98
	ATOM	1282	N	LEU	469	24.547	17.100	-0.011	1.00	42.33
	ATOM	1283	CA	LEU	469	23.890	18.301	0.486	1.00	40.42
	ATOM	1284	CB	LEU	469	24.002	19.427	-0.545	1.00	44.47
	ATOM	1285	CG	LEU	469	25.438	19.874	-0.849	1.00	46.70
50	ATOM	1286	CD1	LEU	469	25.514	20.477	-2.246	1.00	46.70
	ATOM	1287	CD2	LEU	469	25.890	20.883	0.199	1.00	47.32
	ATOM	1288	C	LEU	469	22.423	17.996	0.786	1.00	39.06
	ATOM	1289	O	LEU	469	21.856	18.505	1.760	1.00	34.97
	ATOM	1290	N	GLU	470	21.814	17.151	-0.046	1.00	35.46
55	ATOM	1291	CA	GLU	470	20.418	16.768	0.145	1.00	34.38
	ATOM	1292	CB	GLU	470	19.914	15.963	-1.052	1.00	38.02
	ATOM	1293	CG	GLU	470	19.772	16.773	-2.329	1.00	42.67
	ATOM	1294	CD	GLU	470	19.339	15.923	-3.509	1.00	48.30
	ATOM	1295	OE1	GLU	470	19.671	14.716	-3.538	1.00	50.53
60	ATOM	1296	OE2	GLU	470	18.666	16.463	-4.412	1.00	51.06
	ATOM	1297	C	GLU	470	20.290	15.916	1.403	1.00	34.37

5	ATOM	1298	O	GLU	470	19.321	16.035	2.157	1.00	32.60
	ATOM	1299	N	GLU	471	21.274	15.046	1.606	1.00	34.66
	ATOM	1300	CA	GLU	471	21.309	14.162	2.766	1.00	35.68
	ATOM	1301	CB	GLU	471	22.515	13.222	2.671	1.00	34.57
	ATOM	1302	CG	GLU	471	22.376	12.122	1.614	1.00	37.98
10	ATOM	1303	CD	GLU	471	21.476	10.989	2.063	1.00	39.79
	ATOM	1304	OE1	GLU	471	20.268	11.027	1.743	1.00	41.12
	ATOM	1305	OE2	GLU	471	21.974	10.061	2.737	1.00	32.11
	ATOM	1306	C	GLU	471	21.393	14.983	4.052	1.00	34.79
	ATOM	1307	O	GLU	471	20.596	14.793	4.969	1.00	32.80
15	ATOM	1308	N	LYS	472	22.358	15.898	4.112	1.00	33.93
	ATOM	1309	CA	LYS	472	22.518	16.739	5.291	1.00	35.58
	ATOM	1310	CB	LYS	472	23.683	17.710	5.097	1.00	39.11
	ATOM	1311	CG	LYS	472	25.050	17.050	5.138	1.00	41.47
	ATOM	1312	CD	LYS	472	26.080	17.957	5.794	1.00	46.97
20	ATOM	1313	CE	LYS	472	27.445	17.286	5.862	1.00	48.40
	ATOM	1314	NZ	LYS	472	27.850	16.702	4.547	1.00	51.55
	ATOM	1315	C	LYS	472	21.237	17.523	5.582	1.00	34.78
	ATOM	1316	O	LYS	472	20.795	17.607	6.724	1.00	33.95
	ATOM	1317	N	ASP	473	20.643	18.097	4.545	1.00	33.47
25	ATOM	1318	CA	ASP	473	19.420	18.865	4.720	1.00	34.63
	ATOM	1319	CB	ASP	473	18.923	19.404	3.380	1.00	37.21
	ATOM	1320	CG	ASP	473	17.654	20.221	3.522	1.00	43.24
	ATOM	1321	OD1	ASP	473	16.559	19.687	3.230	1.00	45.20
	ATOM	1322	OD2	ASP	473	17.750	21.396	3.932	1.00	45.59
30	ATOM	1323	C	ASP	473	18.339	17.998	5.338	1.00	32.93
	ATOM	1324	O	ASP	473	17.642	18.416	6.264	1.00	32.87
	ATOM	1325	N	HIS	474	18.199	16.784	4.827	1.00	32.74
	ATOM	1326	CA	HIS	474	17.185	15.882	5.343	1.00	32.21
	ATOM	1327	CB	HIS	474	17.185	14.575	4.568	1.00	32.79
35	ATOM	1328	CG	HIS	474	16.047	13.675	4.924	1.00	36.22
	ATOM	1329	CD2	HIS	474	14.711	13.813	4.750	1.00	38.33
	ATOM	1330	ND1	HIS	474	16.227	12.456	5.542	1.00	38.97
	ATOM	1331	CE1	HIS	474	15.053	11.883	5.732	1.00	37.99
	ATOM	1332	NE2	HIS	474	14.116	12.686	5.261	1.00	37.43
40	ATOM	1333	C	HIS	474	17.403	15.573	6.815	1.00	29.74
	ATOM	1334	O	HIS	474	16.460	15.543	7.596	1.00	29.90
	ATOM	1335	N	ILE	475	18.653	15.326	7.185	1.00	27.80
	ATOM	1336	CA	ILE	475	18.971	15.014	8.571	1.00	25.61
	ATOM	1337	CB	ILE	475	20.478	14.708	8.720	1.00	25.59
45	ATOM	1338	CG2	ILE	475	20.877	14.713	10.193	1.00	27.17
	ATOM	1339	CG1	ILE	475	20.787	13.341	8.092	1.00	26.17
	ATOM	1340	CD1	ILE	475	22.258	13.071	7.849	1.00	27.07
	ATOM	1341	C	ILE	475	18.576	16.201	9.460	1.00	27.91
	ATOM	1342	O	ILE	475	17.928	16.038	10.485	1.00	29.16
50	ATOM	1343	N	HIS	476	18.956	17.404	9.054	1.00	29.41
	ATOM	1344	CA	HIS	476	18.621	18.575	9.846	1.00	29.73
	ATOM	1345	CB	HIS	476	19.342	19.796	9.281	1.00	32.27
	ATOM	1346	CG	HIS	476	20.777	19.867	9.699	1.00	39.44
	ATOM	1347	CD2	HIS	476	21.355	19.707	10.915	1.00	39.81
55	ATOM	1348	ND1	HIS	476	21.809	20.067	8.808	1.00	39.79
	ATOM	1349	CE1	HIS	476	22.959	20.027	9.456	1.00	39.98
	ATOM	1350	NE2	HIS	476	22.712	19.809	10.735	1.00	40.26
	ATOM	1351	C	HIS	476	17.120	18.810	9.948	1.00	31.40
	ATOM	1352	O	HIS	476	16.636	19.336	10.951	1.00	29.79
60	ATOM	1353	N	ARG	477	16.374	18.396	8.929	1.00	31.82
	ATOM	1354	CA	ARG	477	14.929	18.570	8.956	1.00	31.53

5	ATOM	1355	CB	ARG	477	14.343	18.376	7.557	1.00	34.95
	ATOM	1356	CG	ARG	477	14.425	19.627	6.700	1.00	40.46
	ATOM	1357	CD	ARG	477	13.698	19.445	5.370	1.00	45.22
	ATOM	1358	NE	ARG	477	14.107	20.456	4.399	1.00	53.05
	ATOM	1359	CZ	ARG	477	13.647	21.705	4.376	1.00	55.89
10	ATOM	1360	NH1	ARG	477	12.756	22.106	5.274	1.00	56.17
	ATOM	1361	NH2	ARG	477	14.084	22.558	3.457	1.00	59.49
	ATOM	1362	C	ARG	477	14.310	17.582	9.931	1.00	30.70
	ATOM	1363	O	ARG	477	13.360	17.903	10.649	1.00	30.24
	ATOM	1364	N	VAL	478	14.863	16.375	9.972	1.00	29.67
15	ATOM	1365	CA	VAL	478	14.351	15.369	10.887	1.00	29.68
	ATOM	1366	CB	VAL	478	14.937	13.975	10.575	1.00	32.01
	ATOM	1367	CG1	VAL	478	14.461	12.973	11.609	1.00	32.93
	ATOM	1368	CG2	VAL	478	14.506	13.528	9.169	1.00	31.00
	ATOM	1369	C	VAL	478	14.696	15.774	12.316	1.00	29.81
20	ATOM	1370	O	VAL	478	13.860	15.677	13.220	1.00	30.25
	ATOM	1371	N	LEU	479	15.929	16.232	12.516	1.00	28.81
	ATOM	1372	CA	LEU	479	16.360	16.674	13.836	1.00	28.74
	ATOM	1373	CB	LEU	479	17.799	17.210	13.779	1.00	26.65
	ATOM	1374	CG	LEU	479	18.910	16.152	13.853	1.00	26.05
25	ATOM	1375	CD1	LEU	479	20.231	16.772	13.395	1.00	25.81
	ATOM	1376	CD2	LEU	479	19.028	15.603	15.277	1.00	25.34
	ATOM	1377	C	LEU	479	15.411	17.777	14.313	1.00	29.54
	ATOM	1378	O	LEU	479	14.997	17.786	15.472	1.00	29.00
	ATOM	1379	N	ASP	480	15.076	18.703	13.415	1.00	31.52
30	ATOM	1380	CA	ASP	480	14.162	19.800	13.741	1.00	33.84
	ATOM	1381	CB	ASP	480	13.943	20.712	12.528	1.00	34.37
	ATOM	1382	CG	ASP	480	15.055	21.743	12.345	1.00	36.26
	ATOM	1383	OD1	ASP	480	15.119	22.354	11.257	1.00	36.56
	ATOM	1384	OD2	ASP	480	15.860	21.951	13.274	1.00	34.19
35	ATOM	1385	C	ASP	480	12.818	19.222	14.174	1.00	33.48
	ATOM	1386	O	ASP	480	12.186	19.724	15.105	1.00	33.89
	ATOM	1387	N	LYS	481	12.379	18.161	13.498	1.00	33.90
	ATOM	1388	CA	LYS	481	11.106	17.536	13.839	1.00	32.97
	ATOM	1389	CB	LYS	481	10.719	16.489	12.784	1.00	34.66
40	ATOM	1390	C	LYS	481	11.164	16.895	15.225	1.00	33.57
	ATOM	1391	O	LYS	481	10.167	16.869	15.943	1.00	35.37
	ATOM	1392	N	ILE	482	12.328	16.377	15.607	1.00	32.71
	ATOM	1393	CA	ILE	482	12.457	15.764	16.922	1.00	31.60
	ATOM	1394	CB	ILE	482	13.743	14.913	17.028	1.00	32.65
45	ATOM	1395	CG2	ILE	482	13.877	14.338	18.430	1.00	32.50
	ATOM	1396	CG1	ILE	482	13.697	13.785	15.995	1.00	32.72
	ATOM	1397	CD1	ILE	482	14.978	12.969	15.908	1.00	33.37
	ATOM	1398	C	ILE	482	12.456	16.853	17.994	1.00	31.69
	ATOM	1399	O	ILE	482	11.946	16.649	19.097	1.00	29.98
50	ATOM	1400	N	THR	483	13.027	18.012	17.679	1.00	31.33
	ATOM	1401	CA	THR	483	13.022	19.109	18.644	1.00	31.71
	ATOM	1402	CB	THR	483	13.756	20.351	18.109	1.00	32.92
	ATOM	1403	OG1	THR	483	15.111	20.012	17.788	1.00	29.99
	ATOM	1404	CG2	THR	483	13.756	21.452	19.160	1.00	30.47
55	ATOM	1405	C	THR	483	11.559	19.483	18.920	1.00	32.85
	ATOM	1406	O	THR	483	11.146	19.598	20.070	1.00	31.83
	ATOM	1407	N	ASP	484	10.785	19.656	17.851	1.00	31.91
	ATOM	1408	CA	ASP	484	9.369	20.003	17.965	1.00	34.15
	ATOM	1409	CB	ASP	484	8.708	20.013	16.591	1.00	37.41
60	ATOM	1410	CG	ASP	484	9.270	21.080	15.680	1.00	42.02
	ATOM	1411	OD1	ASP	484	9.871	22.045	16.198	1.00	43.26

5	ATOM	1412	OD2	ASP	484	9.106	20.952	14.445	1.00	42.49
	ATOM	1413	C	ASP	484	8.657	18.985	18.840	1.00	33.16
	ATOM	1414	O	ASP	484	7.830	19.339	19.676	1.00	34.86
	ATOM	1415	N	THR	485	8.996	17.715	18.646	1.00	33.91
	ATOM	1416	CA	THR	485	8.396	16.635	19.414	1.00	34.41
10	ATOM	1417	CB	THR	485	8.875	15.268	18.885	1.00	33.58
	ATOM	1418	OG1	THR	485	8.400	15.094	17.542	1.00	37.04
	ATOM	1419	CG2	THR	485	8.347	14.138	19.751	1.00	30.89
	ATOM	1420	C	THR	485	8.708	16.757	20.903	1.00	35.15
	ATOM	1421	O	THR	485	7.818	16.600	21.744	1.00	31.99
15	ATOM	1422	N	LEU	486	9.966	17.046	21.229	1.00	33.77
	ATOM	1423	CA	LEU	486	10.368	17.192	22.621	1.00	34.31
	ATOM	1424	CB	LEU	486	11.879	17.448	22.721	1.00	32.00
	ATOM	1425	CG	LEU	486	12.776	16.201	22.754	1.00	34.99
	ATOM	1426	CD1	LEU	486	14.233	16.613	22.521	1.00	32.65
20	ATOM	1427	CD2	LEU	486	12.635	15.481	24.105	1.00	29.90
	ATOM	1428	C	LEU	486	9.597	18.348	23.256	1.00	34.87
	ATOM	1429	O	LEU	486	9.078	18.225	24.362	1.00	35.85
	ATOM	1430	N	ILE	487	9.513	19.469	22.548	1.00	35.59
	ATOM	1431	CA	ILE	487	8.787	20.625	23.064	1.00	36.79
25	ATOM	1432	CB	ILE	487	8.890	21.826	22.095	1.00	37.32
	ATOM	1433	CG2	ILE	487	7.833	22.884	22.443	1.00	40.19
	ATOM	1434	CG1	ILE	487	10.292	22.443	22.181	1.00	36.00
	ATOM	1435	CD1	ILE	487	10.635	23.041	23.544	1.00	33.58
	ATOM	1436	C	ILE	487	7.315	20.257	23.276	1.00	38.56
30	ATOM	1437	O	ILE	487	6.708	20.628	24.282	1.00	38.52
	ATOM	1438	N	HIS	488	6.749	19.521	22.326	1.00	40.33
	ATOM	1439	CA	HIS	488	5.357	19.096	22.427	1.00	42.29
	ATOM	1440	CB	HIS	488	4.962	18.282	21.197	1.00	44.26
	ATOM	1441	CG	HIS	488	3.612	17.647	21.305	1.00	47.75
35	ATOM	1442	CD2	HIS	488	2.369	18.175	21.214	1.00	47.46
	ATOM	1443	ND1	HIS	488	3.440	16.298	21.534	1.00	51.09
	ATOM	1444	CE1	HIS	488	2.148	16.023	21.577	1.00	51.15
	ATOM	1445	NE2	HIS	488	1.477	17.144	21.385	1.00	50.22
	ATOM	1446	C	HIS	488	5.154	18.254	23.685	1.00	42.55
40	ATOM	1447	O	HIS	488	4.233	18.498	24.467	1.00	43.02
	ATOM	1448	N	LEU	489	6.022	17.266	23.879	1.00	39.91
	ATOM	1449	CA	LEU	489	5.936	16.399	25.048	1.00	39.93
	ATOM	1450	CB	LEU	489	7.087	15.396	25.048	1.00	38.83
	ATOM	1451	CG	LEU	489	6.961	14.242	24.056	1.00	39.31
45	ATOM	1452	CD1	LEU	489	8.259	13.456	24.027	1.00	39.01
	ATOM	1453	CD2	LEU	489	5.799	13.345	24.459	1.00	41.98
	ATOM	1454	C	LEU	489	5.973	17.203	26.339	1.00	40.24
	ATOM	1455	O	LEU	489	5.267	16.888	27.298	1.00	38.72
	ATOM	1456	N	MET	490	6.798	18.246	26.353	1.00	39.94
50	ATOM	1457	CA	MET	490	6.939	19.102	27.522	1.00	41.50
	ATOM	1458	CB	MET	490	8.208	19.953	27.394	1.00	39.15
	ATOM	1459	CG	MET	490	9.495	19.169	27.608	1.00	41.69
	ATOM	1460	SD	MET	490	10.978	20.106	27.161	1.00	35.76
	ATOM	1461	CE	MET	490	12.178	18.775	27.056	1.00	39.22
55	ATOM	1462	C	MET	490	5.718	20.004	27.717	1.00	42.33
	ATOM	1463	O	MET	490	5.296	20.258	28.848	1.00	41.09
	ATOM	1464	N	ALA	491	5.162	20.498	26.616	1.00	43.15
	ATOM	1465	CA	ALA	491	3.983	21.351	26.693	1.00	43.79
	ATOM	1466	CB	ALA	491	3.622	21.879	25.311	1.00	43.93
60	ATOM	1467	C	ALA	491	2.841	20.510	27.251	1.00	46.16
	ATOM	1468	O	ALA	491	2.073	20.967	28.095	1.00	44.69

5	ATOM	1469	N	LYS	492	2.752	19.268	26.783	1.00	46.29
	ATOM	1470	CA	LYS	492	1.711	18.351	27.222	1.00	49.90
	ATOM	1471	CB	LYS	492	1.772	17.053	26.411	1.00	50.03
	ATOM	1472	CG	LYS	492	1.087	17.135	25.062	1.00	53.81
	ATOM	1473	CD	LYS	492	-0.002	16.084	24.930	1.00	59.00
10	ATOM	1474	CE	LYS	492	-0.988	16.453	23.827	1.00	61.85
	ATOM	1475	NZ	LYS	492	-1.351	15.281	22.976	1.00	62.89
	ATOM	1476	C	LYS	492	1.841	18.025	28.701	1.00	51.15
	ATOM	1477	O	LYS	492	0.845	17.784	29.379	1.00	53.37
	ATOM	1478	N	ALA	493	3.072	18.012	29.199	1.00	50.15
15	ATOM	1479	CA	ALA	493	3.321	17.706	30.600	1.00	49.17
	ATOM	1480	CB	ALA	493	4.777	17.314	30.794	1.00	50.39
	ATOM	1481	C	ALA	493	2.971	18.885	31.501	1.00	49.36
	ATOM	1482	O	ALA	493	3.089	18.799	32.723	1.00	51.57
	ATOM	1483	N	GLY	494	2.554	19.989	30.893	1.00	48.61
20	ATOM	1484	CA	GLY	494	2.185	21.159	31.671	1.00	46.92
	ATOM	1485	C	GLY	494	3.322	22.107	32.006	1.00	45.46
	ATOM	1486	O	GLY	494	3.206	22.921	32.919	1.00	43.58
	ATOM	1487	N	LEU	495	4.431	22.009	31.284	1.00	44.81
	ATOM	1488	CA	LEU	495	5.555	22.899	31.540	1.00	42.34
25	ATOM	1489	CB	LEU	495	6.847	22.293	30.988	1.00	43.79
	ATOM	1490	CG	LEU	495	7.712	21.459	31.936	1.00	40.99
	ATOM	1491	CD1	LEU	495	7.022	20.156	32.260	1.00	44.70
	ATOM	1492	CD2	LEU	495	9.072	21.189	31.270	1.00	42.12
	ATOM	1493	C	LEU	495	5.278	24.227	30.847	1.00	42.13
30	ATOM	1494	O	LEU	495	4.664	24.258	29.778	1.00	42.49
	ATOM	1495	N	THR	496	5.718	25.324	31.452	1.00	42.73
	ATOM	1496	CA	THR	496	5.521	26.636	30.845	1.00	43.56
	ATOM	1497	CB	THR	496	5.841	27.767	31.829	1.00	46.09
	ATOM	1498	OG1	THR	496	7.222	27.688	32.208	1.00	43.92
35	ATOM	1499	CG2	THR	496	4.965	27.662	33.064	1.00	45.63
	ATOM	1500	C	THR	496	6.471	26.764	29.660	1.00	45.54
	ATOM	1501	O	THR	496	7.370	25.939	29.488	1.00	43.39
	ATOM	1502	N	LEU	497	6.280	27.800	28.849	1.00	45.02
	ATOM	1503	CA	LEU	497	7.135	28.020	27.688	1.00	45.12
40	ATOM	1504	CB	LEU	497	6.710	29.286	26.944	1.00	46.62
	ATOM	1505	CG	LEU	497	5.933	29.080	25.640	1.00	50.20
	ATOM	1506	CD1	LEU	497	5.886	30.397	24.875	1.00	50.95
	ATOM	1507	CD2	LEU	497	6.589	27.990	24.798	1.00	50.91
	ATOM	1508	C	LEU	497	8.599	28.135	28.101	1.00	44.94
45	ATOM	1509	O	LEU	497	9.474	27.516	27.493	1.00	45.03
	ATOM	1510	N	GLN	498	8.862	28.927	29.137	1.00	41.14
	ATOM	1511	CA	GLN	498	10.221	29.101	29.627	1.00	40.54
	ATOM	1512	CB	GLN	498	10.246	30.140	30.743	1.00	43.82
	ATOM	1513	CG	GLN	498	11.585	30.270	31.437	1.00	43.37
50	ATOM	1514	CD	GLN	498	11.539	31.260	32.584	1.00	47.03
	ATOM	1515	OE1	GLN	498	10.565	31.308	33.332	1.00	49.18
	ATOM	1516	NE2	GLN	498	12.591	32.054	32.727	1.00	45.30
	ATOM	1517	C	GLN	498	10.777	27.773	30.145	1.00	39.39
	ATOM	1518	O	GLN	498	11.923	27.422	29.866	1.00	35.05
55	ATOM	1519	N	GLN	499	9.965	27.040	30.902	1.00	36.49
	ATOM	1520	CA	GLN	499	10.391	25.748	31.434	1.00	36.91
	ATOM	1521	CB	GLN	499	9.314	25.155	32.344	1.00	38.84
	ATOM	1522	CG	GLN	499	9.155	25.825	33.703	1.00	41.33
	ATOM	1523	CD	GLN	499	8.039	25.187	34.512	1.00	42.74
60	ATOM	1524	OE1	GLN	499	7.027	24.760	33.955	1.00	45.44
	ATOM	1525	NE2	GLN	499	8.222	25.107	35.829	1.00	43.48

5	ATOM	1526	C	GLN	499	10.655	24.773	30.285	1.00	35.03
	ATOM	1527	O	GLN	499	11.446	23.832	30.422	1.00	36.59
	ATOM	1528	N	GLN	500	9.980	24.994	29.162	1.00	34.14
	ATOM	1529	CA	GLN	500	10.136	24.138	27.990	1.00	34.65
	ATOM	1530	CB	GLN	500	9.042	24.436	26.958	1.00	33.90
10	ATOM	1531	CG	GLN	500	7.672	23.872	27.315	1.00	36.62
	ATOM	1532	CD	GLN	500	6.558	24.419	26.435	1.00	40.17
	ATOM	1533	OE1	GLN	500	6.660	24.417	25.207	1.00	40.22
	ATOM	1534	NE2	GLN	500	5.482	24.886	27.064	1.00	41.82
	ATOM	1535	C	GLN	500	11.511	24.350	27.358	1.00	34.96
15	ATOM	1536	O	GLN	500	12.256	23.387	27.124	1.00	30.79
	ATOM	1537	N	HIS	501	11.835	25.612	27.078	1.00	34.21
	ATOM	1538	CA	HIS	501	13.117	25.966	26.480	1.00	37.42
	ATOM	1539	CB	HIS	501	13.195	27.476	26.246	1.00	43.08
	ATOM	1540	CG	HIS	501	12.043	28.027	25.468	1.00	51.13
20	ATOM	1541	CD2	HIS	501	11.534	27.678	24.263	1.00	53.05
	ATOM	1542	ND1	HIS	501	11.264	29.068	25.926	1.00	54.54
	ATOM	1543	CE1	HIS	501	10.325	29.337	25.037	1.00	54.36
	ATOM	1544	NE2	HIS	501	10.466	28.508	24.018	1.00	55.19
	ATOM	1545	C	HIS	501	14.255	25.543	27.395	1.00	35.79
25	ATOM	1546	O	HIS	501	15.271	24.996	26.945	1.00	36.20
	ATOM	1547	N	GLN	502	14.086	25.799	28.685	1.00	33.90
	ATOM	1548	CA	GLN	502	15.110	25.438	29.650	1.00	32.18
	ATOM	1549	CB	GLN	502	14.740	25.977	31.033	1.00	35.84
	ATOM	1550	CG	GLN	502	14.787	27.498	31.113	1.00	32.66
30	ATOM	1551	CD	GLN	502	14.420	28.028	32.486	1.00	36.62
	ATOM	1552	OE1	GLN	502	14.102	27.262	33.397	1.00	33.99
	ATOM	1553	NE2	GLN	502	14.462	29.348	32.640	1.00	36.22
	ATOM	1554	C	GLN	502	15.340	23.932	29.716	1.00	31.79
	ATOM	1555	O	GLN	502	16.483	23.479	29.769	1.00	28.00
35	ATOM	1556	N	ARG	503	14.266	23.146	29.705	1.00	30.99
	ATOM	1557	CA	ARG	503	14.436	21.704	29.779	1.00	29.91
	ATOM	1558	CB	ARG	503	13.107	21.011	30.052	1.00	32.79
	ATOM	1559	CG	ARG	503	13.258	19.541	30.400	1.00	30.84
	ATOM	1560	CD	ARG	503	11.930	18.935	30.798	1.00	30.61
40	ATOM	1561	NE	ARG	503	12.021	17.490	30.992	1.00	28.50
	ATOM	1562	CZ	ARG	503	12.489	16.908	32.093	1.00	29.00
	ATOM	1563	NH1	ARG	503	12.917	17.640	33.114	1.00	29.85
	ATOM	1564	NH2	ARG	503	12.512	15.583	32.180	1.00	33.73
	ATOM	1565	C	ARG	503	15.051	21.152	28.496	1.00	29.89
45	ATOM	1566	O	ARG	503	15.895	20.259	28.548	1.00	29.69
	ATOM	1567	N	LEU	504	14.624	21.675	27.351	1.00	28.99
	ATOM	1568	CA	LEU	504	15.164	21.223	26.075	1.00	28.90
	ATOM	1569	CB	LEU	504	14.566	22.023	24.916	1.00	27.72
	ATOM	1570	CG	LEU	504	15.327	21.901	23.593	1.00	30.47
50	ATOM	1571	CD1	LEU	504	15.252	20.453	23.117	1.00	31.74
	ATOM	1572	CD2	LEU	504	14.742	22.843	22.542	1.00	29.85
	ATOM	1573	C	LEU	504	16.681	21.419	26.089	1.00	29.69
	ATOM	1574	O	LEU	504	17.439	20.536	25.672	1.00	26.38
	ATOM	1575	N	ALA	505	17.114	22.585	26.564	1.00	28.51
55	ATOM	1576	CA	ALA	505	18.535	22.899	26.632	1.00	25.98
	ATOM	1577	CB	ALA	505	18.735	24.361	27.039	1.00	29.86
	ATOM	1578	C	ALA	505	19.261	21.977	27.604	1.00	26.67
	ATOM	1579	O	ALA	505	20.340	21.462	27.290	1.00	25.54
	ATOM	1580	N	GLN	506	18.677	21.771	28.784	1.00	23.59
60	ATOM	1581	CA	GLN	506	19.299	20.907	29.785	1.00	27.67
	ATOM	1582	CB	GLN	506	18.434	20.796	31.043	1.00	27.75



5	ATOM	1583	CG	GLN	506	18.414	22.027	31.945	1.00	32.48
	ATOM	1584	CD	GLN	506	17.111	22.116	32.736	1.00	38.40
	ATOM	1585	OE1	GLN	506	16.319	21.167	32.754	1.00	35.97
	ATOM	1586	NE2	GLN	506	16.879	23.257	33.386	1.00	38.07
	ATOM	1587	C	GLN	506	19.500	19.509	29.217	1.00	24.53
10	ATOM	1588	O	GLN	506	20.536	18.889	29.441	1.00	26.42
	ATOM	1589	N	LEU	507	18.505	19.017	28.484	1.00	26.78
	ATOM	1590	CA	LEU	507	18.578	17.678	27.902	1.00	26.18
	ATOM	1591	CB	LEU	507	17.225	17.286	27.295	1.00	31.48
	ATOM	1592	CG	LEU	507	16.052	16.961	28.231	1.00	32.59
15	ATOM	1593	CD1	LEU	507	14.836	16.561	27.389	1.00	33.78
	ATOM	1594	CD2	LEU	507	16.431	15.838	29.174	1.00	30.18
	ATOM	1595	C	LEU	507	19.652	17.583	26.819	1.00	26.03
	ATOM	1596	O	LEU	507	20.421	16.621	26.771	1.00	27.28
	ATOM	1597	N	LEU	508	19.713	18.583	25.950	1.00	24.31
20	ATOM	1598	CA	LEU	508	20.690	18.557	24.863	1.00	23.68
	ATOM	1599	CB	LEU	508	20.339	19.629	23.828	1.00	23.91
	ATOM	1600	CG	LEU	508	19.004	19.436	23.102	1.00	24.68
	ATOM	1601	CD1	LEU	508	18.905	20.416	21.945	1.00	25.11
	ATOM	1602	CD2	LEU	508	18.903	17.994	22.580	1.00	27.53
25	ATOM	1603	C	LEU	508	22.127	18.727	25.341	1.00	22.93
	ATOM	1604	O	LEU	508	23.062	18.200	24.736	1.00	21.36
	ATOM	1605	N	LEU	509	22.302	19.451	26.441	1.00	23.86
	ATOM	1606	CA	LEU	509	23.637	19.661	26.991	1.00	26.28
	ATOM	1607	CB	LEU	509	23.598	20.735	28.095	1.00	28.08
30	ATOM	1608	CG	LEU	509	23.578	22.214	27.672	1.00	33.98
	ATOM	1609	CD1	LEU	509	23.529	23.114	28.921	1.00	35.23
	ATOM	1610	CD2	LEU	509	24.818	22.525	26.856	1.00	30.48
	ATOM	1611	C	LEU	509	24.154	18.327	27.540	1.00	26.08
	ATOM	1612	O	LEU	509	25.354	18.068	27.547	1.00	23.92
35	ATOM	1613	N	ILE	510	23.254	17.462	27.993	1.00	24.60
	ATOM	1614	CA	ILE	510	23.712	16.172	28.496	1.00	25.12
	ATOM	1615	CB	ILE	510	22.568	15.368	29.161	1.00	28.51
	ATOM	1616	CG2	ILE	510	23.051	13.965	29.506	1.00	31.67
	ATOM	1617	CG1	ILE	510	22.141	16.060	30.459	1.00	31.18
40	ATOM	1618	CD1	ILE	510	20.712	15.749	30.882	1.00	37.16
	ATOM	1619	C	ILE	510	24.337	15.351	27.364	1.00	23.86
	ATOM	1620	O	ILE	510	25.225	14.534	27.600	1.00	24.14
	ATOM	1621	N	LEU	511	23.889	15.586	26.133	1.00	25.10
	ATOM	1622	CA	LEU	511	24.420	14.862	24.977	1.00	25.63
45	ATOM	1623	CB	LEU	511	23.628	15.225	23.714	1.00	23.89
	ATOM	1624	CG	LEU	511	22.152	14.801	23.659	1.00	25.78
	ATOM	1625	CD1	LEU	511	21.648	14.920	22.224	1.00	26.55
	ATOM	1626	CD2	LEU	511	21.990	13.363	24.146	1.00	26.29
	ATOM	1627	C	LEU	511	25.912	15.152	24.771	1.00	27.10
50	ATOM	1628	O	LEU	511	26.641	14.332	24.214	1.00	24.98
	ATOM	1629	N	SER	512	26.372	16.319	25.213	1.00	24.75
	ATOM	1630	CA	SER	512	27.787	16.637	25.076	1.00	23.68
	ATOM	1631	CB	SER	512	28.023	18.129	25.358	1.00	26.12
	ATOM	1632	OG	SER	512	29.271	18.327	25.986	1.00	37.17
55	ATOM	1633	C	SER	512	28.594	15.765	26.050	1.00	23.15
	ATOM	1634	O	SER	512	29.742	15.383	25.769	1.00	22.15
	ATOM	1635	N	AHIS	513	27.993	15.456	27.192	0.50	21.53
	ATOM	1636	N	BHIS	513	28.008	15.453	27.202	0.50	20.99
	ATOM	1637	CA	AHIS	513	28.645	14.624	28.196	0.50	21.79
60	ATOM	1638	CA	BHIS	513	28.696	14.607	28.174	0.50	20.94
	ATOM	1639	CB	AHIS	513	27.920	14.776	29.536	0.50	23.59

5	ATOM	1640	CB	BHIS	513	27.991	14.636	29.536	0.50	21.59
	ATOM	1641	CG	AHIS	513	28.145	16.109	30.179	0.50	27.34
	ATOM	1642	CG	BHIS	513	28.800	14.032	30.642	0.50	23.94
	ATOM	1643	CD2	AHIS	513	29.223	16.616	30.824	0.50	27.56
	ATOM	1644	CD2	BHIS	513	30.095	14.211	31.001	0.50	24.22
10	ATOM	1645	ND1	AHIS	513	27.204	17.117	30.160	0.50	30.62
	ATOM	1646	ND1	BHIS	513	28.285	13.105	31.523	0.50	27.00
	ATOM	1647	CE1	AHIS	513	27.693	18.185	30.763	0.50	26.32
	ATOM	1648	CE1	BHIS	513	29.225	12.740	32.376	0.50	24.40
	ATOM	1649	NE2	AHIS	513	28.916	17.908	31.176	0.50	28.30
15	ATOM	1650	NE2	BHIS	513	30.334	13.396	32.081	0.50	25.54
	ATOM	1651	C	AHIS	513	28.666	13.164	27.738	0.50	19.81
	ATOM	1652	C	BHIS	513	28.720	13.171	27.652	0.50	19.42
	ATOM	1653	O	AHIS	513	29.601	12.426	28.026	0.50	22.45
	ATOM	1654	O	BHIS	513	29.707	12.457	27.809	0.50	22.62
20	ATOM	1655	N	ILE	514	27.633	12.753	27.015	1.00	20.76
	ATOM	1656	CA	ILE	514	27.572	11.396	26.492	1.00	20.94
	ATOM	1657	CB	ILE	514	26.154	11.086	25.953	1.00	27.76
	ATOM	1658	CG2	ILE	514	26.169	9.800	25.123	1.00	28.26
	ATOM	1659	CG1	ILE	514	25.185	10.965	27.139	1.00	27.91
25	ATOM	1660	CD1	ILE	514	23.752	10.649	26.753	1.00	34.31
	ATOM	1661	C	ILE	514	28.641	11.256	25.398	1.00	20.66
	ATOM	1662	O	ILE	514	29.298	10.226	25.285	1.00	22.21
	ATOM	1663	N	ARG	515	28.825	12.294	24.589	1.00	20.48
	ATOM	1664	CA	ARG	515	29.861	12.243	23.554	1.00	21.98
30	ATOM	1665	CB	ARG	515	29.861	13.535	22.726	1.00	23.11
	ATOM	1666	CG	ARG	515	31.003	13.611	21.737	1.00	25.76
	ATOM	1667	CD	ARG	515	30.664	12.818	20.491	1.00	28.55
	ATOM	1668	NE	ARG	515	29.580	13.482	19.788	1.00	36.24
	ATOM	1669	CZ	ARG	515	29.615	13.827	18.508	1.00	38.91
35	ATOM	1670	NH1	ARG	515	30.689	13.566	17.776	1.00	35.37
	ATOM	1671	NH2	ARG	515	28.579	14.459	17.971	1.00	40.27
	ATOM	1672	C	ARG	515	31.221	12.087	24.225	1.00	21.29
	ATOM	1673	O	ARG	515	32.068	11.305	23.795	1.00	20.06
	ATOM	1674	N	HIS	516	31.420	12.844	25.293	1.00	23.23
40	ATOM	1675	CA	HIS	516	32.675	12.812	26.034	1.00	24.75
	ATOM	1676	CB	HIS	516	32.566	13.794	27.206	1.00	24.03
	ATOM	1677	CG	HIS	516	33.826	13.948	27.990	1.00	31.42
	ATOM	1678	CD2	HIS	516	34.138	13.587	29.257	1.00	35.87
	ATOM	1679	ND1	HIS	516	34.938	14.586	27.489	1.00	33.59
45	ATOM	1680	CE1	HIS	516	35.882	14.613	28.411	1.00	35.70
	ATOM	1681	NE2	HIS	516	35.422	14.013	29.495	1.00	33.35
	ATOM	1682	C	HIS	516	32.965	11.390	26.537	1.00	24.02
	ATOM	1683	O	HIS	516	34.059	10.852	26.362	1.00	23.66
	ATOM	1684	N	MET	517	31.969	10.786	27.168	1.00	20.91
50	ATOM	1685	CA	MET	517	32.109	9.436	27.684	1.00	24.21
	ATOM	1686	CB	MET	517	30.837	9.038	28.424	1.00	23.88
	ATOM	1687	CG	MET	517	30.607	9.903	29.652	1.00	26.32
	ATOM	1688	SD	MET	517	29.435	9.222	30.790	1.00	26.67
	ATOM	1689	CE	MET	517	27.914	9.390	29.807	1.00	23.26
55	ATOM	1690	C	MET	517	32.399	8.448	26.564	1.00	23.26
	ATOM	1691	O	MET	517	33.213	7.547	26.728	1.00	26.08
	ATOM	1692	N	SER	518	31.736	8.612	25.423	1.00	21.93
	ATOM	1693	CA	SER	518	31.977	7.717	24.301	1.00	23.08
	ATOM	1694	CB	SER	518	30.976	8.027	23.173	1.00	22.02
60	ATOM	1695	OG	SER	518	31.283	7.336	21.978	1.00	24.01
	ATOM	1696	C	SER	518	33.432	7.862	23.810	1.00	25.15

5	ATOM	1697	O	SER	518	34.111	6.866	23.532	1.00	22.94
	ATOM	1698	N	ASN	519	33.923	9.097	23.713	1.00	22.42
	ATOM	1699	CA	ASN	519	35.295	9.309	23.260	1.00	21.87
	ATOM	1700	CB	ASN	519	35.605	10.807	23.157	1.00	24.46
	ATOM	1701	CG	ASN	519	34.864	11.469	22.021	1.00	29.02
10	ATOM	1702	OD1	ASN	519	34.661	10.864	20.965	1.00	31.93
	ATOM	1703	ND2	ASN	519	34.459	12.715	22.224	1.00	28.81
	ATOM	1704	C	ASN	519	36.292	8.643	24.201	1.00	21.46
	ATOM	1705	O	ASN	519	37.251	8.015	23.752	1.00	23.56
	ATOM	1706	N	LYS	520	36.070	8.782	25.504	1.00	23.23
15	ATOM	1707	CA	LYS	520	36.964	8.171	26.488	1.00	26.35
	ATOM	1708	CB	LYS	520	36.581	8.592	27.912	1.00	27.53
	ATOM	1709	CG	LYS	520	36.618	10.101	28.174	1.00	33.74
	ATOM	1710	CD	LYS	520	37.962	10.710	27.811	1.00	42.09
	ATOM	1711	CE	LYS	520	39.047	10.307	28.802	1.00	43.97
20	ATOM	1712	NZ	LYS	520	39.858	11.480	29.254	1.00	48.07
	ATOM	1713	C	LYS	520	36.899	6.644	26.376	1.00	27.71
	ATOM	1714	O	LYS	520	37.913	5.957	26.501	1.00	27.15
	ATOM	1715	N	GLY	521	35.704	6.117	26.141	1.00	25.02
	ATOM	1716	CA	GLY	521	35.562	4.676	26.003	1.00	26.67
25	ATOM	1717	C	GLY	521	36.254	4.168	24.753	1.00	27.06
	ATOM	1718	O	GLY	521	36.924	3.128	24.775	1.00	26.84
	ATOM	1719	N	AMET	522	36.101	4.893	23.650	0.50	25.87
	ATOM	1720	N	BMET	522	36.095	4.908	23.658	0.50	27.62
	ATOM	1721	CA	AMET	522	36.727	4.491	22.401	0.50	27.27
30	ATOM	1722	CA	BMET	522	36.703	4.551	22.384	0.50	30.14
	ATOM	1723	CB	AMET	522	36.267	5.396	21.260	0.50	26.50
	ATOM	1724	CB	BMET	522	36.252	5.525	21.288	0.50	32.46
	ATOM	1725	CG	AMET	522	34.827	5.162	20.866	0.50	25.05
	ATOM	1726	CG	BMET	522	35.681	4.854	20.045	0.50	35.70
35	ATOM	1727	SD	AMET	522	34.585	3.587	20.020	0.50	27.07
	ATOM	1728	SD	BMET	522	34.197	5.672	19.408	0.50	40.01
	ATOM	1729	CE	AMET	522	33.142	4.017	19.031	0.50	31.29
	ATOM	1730	CE	BMET	522	34.733	6.085	17.745	0.50	42.12
	ATOM	1731	C	AMET	522	38.242	4.532	22.512	0.50	28.99
40	ATOM	1732	C	BMET	522	38.224	4.567	22.483	0.50	30.76
	ATOM	1733	O	AMET	522	38.939	3.743	21.870	0.50	31.65
	ATOM	1734	O	BMET	522	38.905	3.793	21.807	0.50	32.87
	ATOM	1735	N	GLU	523	38.749	5.452	23.324	1.00	30.85
	ATOM	1736	CA	GLU	523	40.190	5.576	23.513	1.00	34.09
45	ATOM	1737	CB	GLU	523	40.515	6.725	24.480	1.00	35.59
	ATOM	1738	CG	GLU	523	40.658	8.079	23.784	1.00	43.35
	ATOM	1739	CD	GLU	523	40.560	9.265	24.739	1.00	46.63
	ATOM	1740	OE1	GLU	523	39.832	10.240	24.416	1.00	47.64
	ATOM	1741	OE2	GLU	523	41.212	9.225	25.805	1.00	43.09
50	ATOM	1742	C	GLU	523	40.718	4.260	24.061	1.00	34.62
	ATOM	1743	O	GLU	523	41.733	3.747	23.596	1.00	33.87
	ATOM	1744	N	HIS	524	40.021	3.700	25.042	1.00	36.33
	ATOM	1745	CA	HIS	524	40.455	2.427	25.607	1.00	39.20
	ATOM	1746	CB	HIS	524	39.678	2.093	26.878	1.00	40.75
55	ATOM	1747	CG	HIS	524	40.061	0.774	27.473	1.00	48.10
	ATOM	1748	CD2	HIS	524	41.192	0.376	28.104	1.00	48.56
	ATOM	1749	ND1	HIS	524	39.247	-0.338	27.412	1.00	48.84
	ATOM	1750	CE1	HIS	524	39.859	-1.362	27.978	1.00	50.19
	ATOM	1751	NE2	HIS	524	41.041	-0.956	28.407	1.00	51.61
60	ATOM	1752	C	HIS	524	40.290	1.282	24.613	1.00	38.06
	ATOM	1753	O	HIS	524	41.226	0.521	24.371	1.00	38.18

5	ATOM	1754	N	LEU	525	39.101	1.162	24.034	1.00	36.96
	ATOM	1755	CA	LEU	525	38.831	0.093	23.084	1.00	37.40
	ATOM	1756	CB	LEU	525	37.416	0.241	22.514	1.00	35.89
	ATOM	1757	CG	LEU	525	36.268	0.107	23.527	1.00	33.17
	ATOM	1758	CD1	LEU	525	34.936	0.246	22.811	1.00	31.77
10	ATOM	1759	CD2	LEU	525	36.343	-1.240	24.238	1.00	35.92
	ATOM	1760	C	LEU	525	39.859	0.057	21.954	1.00	41.32
	ATOM	1761	O	LEU	525	40.244	-1.015	21.487	1.00	40.76
	ATOM	1762	N	TYR	526	40.314	1.227	21.522	1.00	43.68
	ATOM	1763	CA	TYR	526	41.300	1.297	20.449	1.00	49.00
15	ATOM	1764	CB	TYR	526	41.376	2.722	19.890	1.00	51.86
	ATOM	1765	CG	TYR	526	42.305	2.878	18.704	1.00	57.70
	ATOM	1766	CD1	TYR	526	41.835	2.718	17.400	1.00	58.93
	ATOM	1767	CE1	TYR	526	42.681	2.875	16.305	1.00	61.21
	ATOM	1768	CD2	TYR	526	43.653	3.200	18.883	1.00	58.58
20	ATOM	1769	CE2	TYR	526	44.510	3.359	17.790	1.00	61.15
	ATOM	1770	CZ	TYR	526	44.016	3.194	16.505	1.00	61.09
	ATOM	1771	OH	TYR	526	44.851	3.343	15.417	1.00	63.79
	ATOM	1772	C	TYR	526	42.671	0.871	20.964	1.00	50.14
	ATOM	1773	O	TYR	526	43.471	0.303	20.223	1.00	50.73
25	ATOM	1774	N	SER	527	42.930	1.139	22.240	1.00	52.72
	ATOM	1775	CA	SER	527	44.205	0.790	22.857	1.00	55.88
	ATOM	1776	CB	SER	527	44.351	1.516	24.199	1.00	55.00
	ATOM	1777	OG	SER	527	43.752	0.788	25.257	1.00	52.46
	ATOM	1778	C	SER	527	44.365	-0.718	23.054	1.00	60.39
30	ATOM	1779	O	SER	527	45.398	-1.185	23.534	1.00	60.43
	ATOM	1780	N	MET	528	43.335	-1.472	22.678	1.00	63.86
	ATOM	1781	CA	MET	528	43.347	-2.929	22.788	1.00	67.95
	ATOM	1782	CB	MET	528	42.534	-3.381	24.008	1.00	67.85
	ATOM	1783	CG	MET	528	41.237	-2.606	24.222	1.00	70.10
35	ATOM	1784	SD	MET	528	39.895	-3.569	24.983	1.00	71.70
	ATOM	1785	CE	MET	528	39.231	-4.412	23.554	1.00	72.57
	ATOM	1786	C	MET	528	42.726	-3.502	21.513	1.00	70.33
	ATOM	1787	O	MET	528	42.170	-4.602	21.513	1.00	72.43
	ATOM	1788	N	LYS	529	42.834	-2.739	20.428	1.00	71.53
40	ATOM	1789	CA	LYS	529	42.274	-3.122	19.136	1.00	72.00
	ATOM	1790	CB	LYS	529	42.508	-2.004	18.119	1.00	71.30
	ATOM	1791	C	LYS	529	42.813	-4.439	18.587	1.00	72.47
	ATOM	1792	O	LYS	529	43.990	-4.762	18.751	1.00	70.37
	ATOM	1793	N	CYS	530	41.932	-5.191	17.930	1.00	74.48
45	ATOM	1794	CA	CYS	530	42.279	-6.474	17.325	1.00	76.67
	ATOM	1795	CB	CYS	530	41.004	-7.245	16.952	1.00	77.23
	ATOM	1796	SG	CYS	530	40.447	-8.491	18.146	1.00	79.38
	ATOM	1797	C	CYS	530	43.098	-6.220	16.065	1.00	78.08
	ATOM	1798	O	CYS	530	43.241	-5.076	15.623	1.00	78.81
50	ATOM	1799	N	LYS	531	43.637	-7.289	15.487	1.00	78.22
	ATOM	1800	CA	LYS	531	44.424	-7.187	14.267	1.00	78.15
	ATOM	1801	CB	LYS	531	45.600	-8.182	14.305	1.00	78.33
	ATOM	1802	C	LYS	531	43.508	-7.467	13.067	1.00	77.93
	ATOM	1803	O	LYS	531	42.549	-6.734	12.839	1.00	78.07
55	ATOM	1804	N	ASN	532	43.784	-8.539	12.328	1.00	77.80
	ATOM	1805	CA	ASN	532	42.984	-8.902	11.152	1.00	77.30
	ATOM	1806	CB	ASN	532	43.550	-10.166	10.521	1.00	77.55
	ATOM	1807	C	ASN	532	41.485	-9.082	11.423	1.00	77.34
	ATOM	1808	O	ASN	532	40.904	-10.123	11.118	1.00	78.13
60	ATOM	1809	N	VAL	533	40.859	-8.055	11.988	1.00	76.13
	ATOM	1810	CA	VAL	533	39.436	-8.098	12.280	1.00	73.77

5	ATOM	1811	CB	VAL	533	39.155	-7.715	13.752	1.00	73.62
	ATOM	1812	CG1	VAL	533	39.690	-6.327	14.047	1.00	73.13
	ATOM	1813	CG2	VAL	533	37.662	-7.782	14.021	1.00	73.14
	ATOM	1814	C	VAL	533	38.685	-7.143	11.352	1.00	72.97
	ATOM	1815	O	VAL	533	39.024	-5.960	11.252	1.00	73.91
10	ATOM	1816	N	VAL	534	37.671	-7.666	10.666	1.00	70.02
	ATOM	1817	CA	VAL	534	36.866	-6.867	9.747	1.00	66.70
	ATOM	1818	CB	VAL	534	35.619	-7.646	9.328	1.00	67.32
	ATOM	1819	C	VAL	534	36.463	-5.541	10.393	1.00	63.87
	ATOM	1820	O	VAL	534	35.895	-5.519	11.486	1.00	63.55
15	ATOM	1821	N	PRO	535	36.756	-4.415	9.719	1.00	60.92
	ATOM	1822	CD	PRO	535	37.424	-4.354	8.408	1.00	61.01
	ATOM	1823	CA	PRO	535	36.424	-3.077	10.229	1.00	56.83
	ATOM	1824	CB	PRO	535	36.867	-2.135	9.107	1.00	58.70
	ATOM	1825	CG	PRO	535	37.023	-3.009	7.893	1.00	61.55
20	ATOM	1826	C	PRO	535	34.944	-2.902	10.571	1.00	52.90
	ATOM	1827	O	PRO	535	34.067	-3.461	9.908	1.00	52.01
	ATOM	1828	N	LEU	536	34.672	-2.120	11.610	1.00	48.60
	ATOM	1829	CA	LEU	536	33.301	-1.874	12.042	1.00	45.08
	ATOM	1830	CB	LEU	536	33.280	-0.796	13.128	1.00	44.35
25	ATOM	1831	CG	LEU	536	32.267	-0.911	14.273	1.00	43.48
	ATOM	1832	CD1	LEU	536	31.919	0.490	14.745	1.00	43.41
	ATOM	1833	CD2	LEU	536	31.022	-1.654	13.835	1.00	39.55
	ATOM	1834	C	LEU	536	32.434	-1.433	10.871	1.00	43.58
	ATOM	1835	O	LEU	536	31.287	-1.862	10.734	1.00	42.14
30	ATOM	1836	N	TYR	537	32.992	-0.575	10.024	1.00	43.02
	ATOM	1837	CA	TYR	537	32.269	-0.066	8.866	1.00	43.34
	ATOM	1838	CB	TYR	537	33.200	0.786	7.997	1.00	44.76
	ATOM	1839	CG	TYR	537	32.483	1.558	6.913	1.00	48.28
	ATOM	1840	CD1	TYR	537	32.190	0.964	5.687	1.00	48.46
35	ATOM	1841	CE1	TYR	537	31.504	1.660	4.693	1.00	52.48
	ATOM	1842	CD2	TYR	537	32.073	2.875	7.123	1.00	49.99
	ATOM	1843	CE2	TYR	537	31.383	3.584	6.135	1.00	53.73
	ATOM	1844	CZ	TYR	537	31.100	2.967	4.924	1.00	54.01
	ATOM	1845	OH	TYR	537	30.401	3.648	3.952	1.00	55.90
40	ATOM	1846	C	TYR	537	31.683	-1.199	8.032	1.00	43.15
	ATOM	1847	O	TYR	537	30.500	-1.191	7.696	1.00	41.54
	ATOM	1848	N	ASP	538	32.521	-2.175	7.702	1.00	44.67
	ATOM	1849	CA	ASP	538	32.097	-3.309	6.893	1.00	45.49
	ATOM	1850	CB	ASP	538	33.322	-4.126	6.479	1.00	51.32
45	ATOM	1851	CG	ASP	538	34.361	-3.284	5.748	1.00	56.17
	ATOM	1852	OD1	ASP	538	35.436	-3.820	5.396	1.00	57.29
	ATOM	1853	OD2	ASP	538	34.097	-2.079	5.526	1.00	59.24
	ATOM	1854	C	ASP	538	31.071	-4.195	7.587	1.00	43.48
	ATOM	1855	O	ASP	538	30.177	-4.738	6.940	1.00	43.95
50	ATOM	1856	N	LEU	539	31.193	-4.345	8.901	1.00	41.57
	ATOM	1857	CA	LEU	539	30.244	-5.157	9.654	1.00	39.11
	ATOM	1858	CB	LEU	539	30.734	-5.351	11.092	1.00	41.88
	ATOM	1859	CG	LEU	539	29.770	-6.065	12.044	1.00	46.11
	ATOM	1860	CD1	LEU	539	29.298	-7.379	11.423	1.00	46.99
55	ATOM	1861	CD2	LEU	539	30.474	-6.319	13.377	1.00	45.76
	ATOM	1862	C	LEU	539	28.891	-4.451	9.651	1.00	36.38
	ATOM	1863	O	LEU	539	27.849	-5.070	9.436	1.00	35.74
	ATOM	1864	N	LEU	540	28.919	-3.146	9.894	1.00	35.50
	ATOM	1865	CA	LEU	540	27.703	-2.336	9.903	1.00	35.59
60	ATOM	1866	CB	LEU	540	28.061	-0.877	10.219	1.00	37.63
	ATOM	1867	CG	LEU	540	27.856	-0.252	11.605	1.00	40.28

5	ATOM	1868	CD1	LEU	540	27.526	-1.299	12.645	1.00	38.55
	ATOM	1869	CD2	LEU	540	29.114	0.506	11.985	1.00	41.04
	ATOM	1870	C	LEU	540	27.060	-2.415	8.510	1.00	35.50
	ATOM	1871	O	LEU	540	25.846	-2.585	8.371	1.00	33.21
	ATOM	1872	N	LEU	541	27.892	-2.289	7.483	1.00	37.01
10	ATOM	1873	CA	LEU	541	27.418	-2.340	6.101	1.00	38.51
	ATOM	1874	CB	LEU	541	28.591	-2.152	5.145	1.00	39.67
	ATOM	1875	CG	LEU	541	28.301	-2.112	3.643	1.00	40.92
	ATOM	1876	CD1	LEU	541	27.184	-1.130	3.348	1.00	42.44
	ATOM	1877	CD2	LEU	541	29.572	-1.716	2.908	1.00	44.18
15	ATOM	1878	C	LEU	541	26.723	-3.676	5.833	1.00	39.75
	ATOM	1879	O	LEU	541	25.616	-3.713	5.297	1.00	36.48
	ATOM	1880	N	GLU	542	27.366	-4.770	6.230	1.00	40.88
	ATOM	1881	CA	GLU	542	26.790	-6.097	6.037	1.00	41.89
	ATOM	1882	CB	GLU	542	27.719	-7.170	6.620	1.00	44.11
20	ATOM	1883	CG	GLU	542	27.010	-8.457	7.052	1.00	50.60
	ATOM	1884	CD	GLU	542	26.434	-9.245	5.887	1.00	55.80
	ATOM	1885	OE1	GLU	542	25.570	-10.117	6.130	1.00	58.81
	ATOM	1886	OE2	GLU	542	26.842	-8.996	4.728	1.00	57.19
	ATOM	1887	C	GLU	542	25.414	-6.195	6.691	1.00	41.58
25	ATOM	1888	O	GLU	542	24.472	-6.720	6.102	1.00	42.82
	ATOM	1889	N	MET	543	25.298	-5.686	7.915	1.00	40.09
	ATOM	1890	CA	MET	543	24.036	-5.731	8.634	1.00	36.43
	ATOM	1891	CB	MET	543	24.270	-5.424	10.111	1.00	39.95
	ATOM	1892	CG	MET	543	25.137	-6.459	10.808	1.00	41.95
30	ATOM	1893	SD	MET	543	24.918	-6.445	12.604	1.00	47.17
	ATOM	1894	CE	MET	543	25.324	-4.749	12.964	1.00	40.88
	ATOM	1895	C	MET	543	23.001	-4.769	8.072	1.00	35.02
	ATOM	1896	O	MET	543	21.808	-5.073	8.048	1.00	35.31
	ATOM	1897	N	LEU	544	23.457	-3.605	7.629	1.00	32.90
35	ATOM	1898	CA	LEU	544	22.559	-2.603	7.074	1.00	36.88
	ATOM	1899	CB	LEU	544	23.225	-1.226	7.111	1.00	34.51
	ATOM	1900	CG	LEU	544	23.268	-0.562	8.490	1.00	31.94
	ATOM	1901	CD1	LEU	544	24.284	0.564	8.478	1.00	32.27
	ATOM	1902	CD2	LEU	544	21.897	-0.029	8.846	1.00	29.02
40	ATOM	1903	C	LEU	544	22.148	-2.941	5.640	1.00	38.94
	ATOM	1904	O	LEU	544	20.971	-2.842	5.294	1.00	39.52
	ATOM	1905	N	ASP	545	23.118	-3.338	4.817	1.00	41.05
	ATOM	1906	CA	ASP	545	22.850	-3.685	3.418	1.00	40.78
	ATOM	1907	CB	ASP	545	24.159	-3.780	2.620	1.00	37.75
45	ATOM	1908	CG	ASP	545	23.922	-3.937	1.120	1.00	35.19
	ATOM	1909	OD1	ASP	545	24.881	-4.265	0.380	1.00	33.48
	ATOM	1910	OD2	ASP	545	22.768	-3.734	0.691	1.00	31.33
	ATOM	1911	C	ASP	545	22.116	-5.015	3.349	1.00	42.87
	ATOM	1912	O	ASP	545	22.681	-6.030	2.929	1.00	44.32
50	ATOM	1913	N	ALA	546	20.853	-5.009	3.755	1.00	43.49
	ATOM	1914	CA	ALA	546	20.069	-6.229	3.746	1.00	46.96
	ATOM	1915	CB	ALA	546	19.213	-6.305	5.006	1.00	47.82
	ATOM	1916	C	ALA	546	19.193	-6.362	2.508	1.00	49.55
	ATOM	1917	O	ALA	546	18.804	-5.368	1.883	1.00	48.75
55	ATOM	1918	N	HIS	547	18.895	-7.606	2.152	1.00	50.98
	ATOM	1919	CA	HIS	547	18.042	-7.884	1.006	1.00	53.77
	ATOM	1920	CB	HIS	547	18.431	-9.223	0.369	1.00	52.69
	ATOM	1921	CG	HIS	547	18.395	-10.382	1.317	1.00	55.05
	ATOM	1922	CD2	HIS	547	17.477	-10.752	2.242	1.00	53.94
60	ATOM	1923	ND1	HIS	547	19.395	-11.329	1.371	1.00	56.23
	ATOM	1924	CE1	HIS	547	19.095	-12.232	2.286	1.00	55.36

5	ATOM	1925	NE2	HIS	547	17.936	-11.906	2.830	1.00	57.01
	ATOM	1926	C	HIS	547	16.603	-7.936	1.518	1.00	55.69
	ATOM	1927	O	HIS	547	16.362	-7.796	2.720	1.00	54.30
	ATOM	1928	N	ARG	548	15.653	-8.139	0.612	1.00	57.00
	ATOM	1929	CA	ARG	548	14.245	-8.212	0.987	1.00	60.65
10	ATOM	1930	CB	ARG	548	13.432	-7.171	0.208	1.00	62.69
	ATOM	1931	CG	ARG	548	14.272	-6.222	-0.637	1.00	67.54
	ATOM	1932	CD	ARG	548	13.448	-5.061	-1.171	1.00	71.92
	ATOM	1933	NE	ARG	548	13.702	-3.826	-0.432	1.00	76.95
	ATOM	1934	CZ	ARG	548	14.864	-3.178	-0.429	1.00	79.04
15	ATOM	1935	NH1	ARG	548	15.891	-3.644	-1.128	1.00	80.66
	ATOM	1936	NH2	ARG	548	15.001	-2.063	0.278	1.00	80.39
	ATOM	1937	C	ARG	548	13.695	-9.608	0.711	1.00	61.65
	ATOM	1938	O	ARG	548	12.500	-9.781	0.466	1.00	62.05
	ATOM	1939	N	LEU	549	14.576	-10.603	0.756	1.00	62.39
20	ATOM	1940	CA	LEU	549	14.188	-11.985	0.507	1.00	64.02
	ATOM	1941	CB	LEU	549	15.433	-12.828	0.195	1.00	62.14
	ATOM	1942	CG	LEU	549	16.461	-12.191	-0.753	1.00	60.76
	ATOM	1943	CD1	LEU	549	17.699	-13.074	-0.878	1.00	57.77
	ATOM	1944	CD2	LEU	549	15.823	-11.972	-2.108	1.00	58.38
25	ATOM	1945	C	LEU	549	13.431	-12.574	1.702	1.00	66.65
	ATOM	1946	O	LEU	549	12.759	-13.600	1.577	1.00	67.15
	ATOM	1947	N	HIS	550	13.541	-11.920	2.856	1.00	67.72
	ATOM	1948	CA	HIS	550	12.858	-12.378	4.065	1.00	69.93
	ATOM	1949	CB	HIS	550	13.753	-12.190	5.298	1.00	70.76
30	ATOM	1950	CG	HIS	550	14.977	-13.054	5.306	1.00	71.50
	ATOM	1951	CD2	HIS	550	15.539	-13.821	4.341	1.00	71.63
	ATOM	1952	ND1	HIS	550	15.793	-13.172	6.411	1.00	71.98
	ATOM	1953	CE1	HIS	550	16.805	-13.972	6.126	1.00	72.04
	ATOM	1954	NE2	HIS	550	16.674	-14.379	4.876	1.00	71.39
35	ATOM	1955	C	HIS	550	11.556	-11.603	4.275	1.00	71.15
	ATOM	1956	O	HIS	550	10.940	-11.684	5.340	1.00	70.66
	ATOM	1957	N	ALA	551	11.143	-10.851	3.258	1.00	72.22
	ATOM	1958	CA	ALA	551	9.919	-10.057	3.338	1.00	73.58
	ATOM	1959	CB	ALA	551	9.904	-9.014	2.221	1.00	73.21
40	ATOM	1960	C	ALA	551	8.658	-10.920	3.266	1.00	74.69
	ATOM	1961	O	ALA	551	7.684	-10.474	2.621	1.00	76.12
	ATOM	1962	OXT	ALA	551	8.651	-12.025	3.852	1.00	73.79
	HETATM	1963	C10	OHT	600	30.581	1.481	29.471	1.00	26.84
	HETATM	1964	C9	OHT	600	30.713	-0.043	29.358	1.00	22.85
45	HETATM	1965	C8	OHT	600	31.366	-0.385	28.037	1.00	25.56
	HETATM	1966	C11	OHT	600	32.761	0.051	27.916	1.00	27.51
	HETATM	1967	C16	OHT	600	33.218	0.797	26.797	1.00	28.35
	HETATM	1968	C15	OHT	600	34.551	1.237	26.747	1.00	30.39
	HETATM	1969	C14	OHT	600	35.443	0.923	27.792	1.00	30.23
50	HETATM	1970	C13	OHT	600	35.004	0.185	28.890	1.00	31.45
	HETATM	1971	C12	OHT	600	33.666	-0.241	28.955	1.00	27.93
	HETATM	1972	C7	OHT	600	30.682	-1.089	27.077	1.00	24.41
	HETATM	1973	C1	OHT	600	29.211	-1.258	27.052	1.00	24.26
	HETATM	1974	C2	OHT	600	28.644	-2.526	26.706	1.00	25.92
55	HETATM	1975	C3	OHT	600	27.254	-2.668	26.580	1.00	26.32
	HETATM	1976	C4	OHT	600	26.438	-1.553	26.813	1.00	29.02
	HETATM	1977	O4	OHT	600	25.072	-1.605	26.716	1.00	28.42
	HETATM	1978	C5	OHT	600	26.980	-0.286	27.130	1.00	26.98
	HETATM	1979	C6	OHT	600	28.362	-0.147	27.231	1.00	25.23
60	HETATM	1980	C17	OHT	600	31.370	-1.692	25.942	1.00	26.61
	HETATM	1981	C18	OHT	600	32.508	-2.498	26.151	1.00	26.77

5	HETATM	1982	C19	OHT	600	33.166	-3.052	25.072	1.00	27.50
	HETATM	1983	C20	OHT	600	32.676	-2.794	23.786	1.00	27.50
	HETATM	1984	O20	OHT	600	33.206	-3.566	22.795	1.00	31.35
	HETATM	1985	C23	OHT	600	33.009	-3.135	21.448	1.00	40.09
	HETATM	1986	C24	OHT	600	34.226	-3.490	20.575	1.00	44.80
10	HETATM	1987	N24	OHT	600	34.141	-4.901	20.203	1.00	49.00
	HETATM	1988	C25	OHT	600	33.375	-5.040	18.933	1.00	51.64
	HETATM	1989	C26	OHT	600	35.495	-5.459	20.004	1.00	52.06
	HETATM	1990	C21	OHT	600	31.540	-2.005	23.558	1.00	27.19
	HETATM	1991	C22	OHT	600	30.892	-1.450	24.645	1.00	27.92
15	HETATM	1992	O1	HOH	1	20.714	-12.010	23.057	1.00	27.20
	HETATM	1993	O1	HOH	2	22.563	-0.070	25.819	1.00	25.77
	HETATM	1994	O1	HOH	3	25.183	19.202	23.149	1.00	42.52
	HETATM	1995	O1	HOH	4	35.158	5.823	37.390	1.00	33.92
	HETATM	1996	O1	HOH	5	22.116	-9.922	18.914	1.00	30.18
20	HETATM	1997	O1	HOH	6	29.812	6.536	19.652	1.00	26.11
	HETATM	1998	O1	HOH	7	13.362	4.463	20.376	1.00	29.40
	HETATM	1999	O1	HOH	8	19.799	-11.295	20.187	1.00	28.70
	HETATM	2000	O1	HOH	9	21.205	1.466	23.794	1.00	22.47
	HETATM	2001	O1	HOH	10	21.177	-4.961	29.066	1.00	33.00
25	HETATM	2002	O1	HOH	11	18.591	1.863	20.518	1.00	32.59
	HETATM	2003	O1	HOH	12	16.298	21.566	15.992	1.00	33.42
	HETATM	2004	O1	HOH	13	18.611	1.976	24.494	1.00	29.70
	HETATM	2005	O1	HOH	14	38.009	8.910	21.156	1.00	39.92
	HETATM	2006	O1	HOH	15	26.549	11.664	18.080	1.00	30.25
30	HETATM	2007	O1	HOH	16	20.282	-4.239	26.512	1.00	32.70
	HETATM	2008	O1	HOH	17	32.858	8.754	20.237	1.00	29.88
	HETATM	2009	O1	HOH	18	8.497	16.136	29.934	1.00	46.80
	HETATM	2010	O1	HOH	19	21.940	19.301	31.632	1.00	35.72
	HETATM	2011	O1	HOH	20	35.153	2.682	14.122	1.00	41.02
35	HETATM	2012	O1	HOH	21	20.358	-2.268	21.013	1.00	29.43
	HETATM	2013	O1	HOH	22	35.562	10.036	36.334	1.00	41.37
	HETATM	2014	O1	HOH	23	17.248	18.187	17.571	1.00	33.96
	HETATM	2015	O1	HOH	24	18.445	20.973	12.346	1.00	43.44
	HETATM	2016	O1	HOH	25	12.152	23.054	33.132	1.00	36.04
40	HETATM	2017	O1	HOH	26	13.181	22.222	9.699	1.00	37.03
	HETATM	2018	O1	HOH	27	19.399	-6.090	12.808	1.00	44.86
	HETATM	2019	O1	HOH	28	37.895	13.599	31.395	1.00	47.26
	HETATM	2020	O1	HOH	29	11.570	6.212	7.962	1.00	51.10
	HETATM	2021	O1	HOH	30	20.172	-2.568	23.445	1.00	51.70
45	HETATM	2022	O1	HOH	31	36.402	-5.369	23.729	1.00	58.20
	HETATM	2023	O1	HOH	32	25.127	13.802	19.187	1.00	35.29
	HETATM	2024	O1	HOH	33	23.181	4.937	38.538	1.00	33.77
	HETATM	2025	O1	HOH	34	20.550	0.421	21.276	1.00	29.12
	HETATM	2026	O1	HOH	35	39.599	13.954	27.312	1.00	44.08
50	HETATM	2027	O1	HOH	36	26.445	13.863	21.285	1.00	34.97
	HETATM	2028	O1	HOH	37	13.759	5.079	9.108	1.00	38.54
	HETATM	2029	O1	HOH	38	14.150	24.731	34.529	1.00	49.72
	HETATM	2030	O1	HOH	39	21.060	13.886	-6.319	1.00	59.79
	HETATM	2031	O1	HOH	40	32.215	6.217	8.726	1.00	60.22
55	HETATM	2032	O1	HOH	41	35.105	15.704	9.069	1.00	45.15
	HETATM	2033	O1	HOH	42	11.427	19.451	9.903	1.00	38.56
	HETATM	2034	O1	HOH	43	19.662	23.472	10.333	1.00	47.71
	HETATM	2035	O1	HOH	44	9.231	3.690	12.337	1.00	45.98
	HETATM	2036	O1	HOH	45	15.313	-6.036	17.192	1.00	39.07
60	HETATM	2037	O1	HOH	46	15.517	-3.266	17.907	1.00	37.67
	HETATM	2038	O1	HOH	47	28.784	-16.713	25.163	1.00	55.44



5	HETATM	2039	01	HOH	48	27.868	-10.898	28.271	1.00	31.27
	HETATM	2040	01	HOH	49	6.955	13.568	28.233	1.00	48.83
	HETATM	2041	01	HOH	50	22.051	-15.030	28.603	1.00	36.91
	HETATM	2042	01	HOH	51	7.026	31.002	30.284	1.00	46.73
	HETATM	2043	01	HOH	52	-1.489	12.385	15.164	1.00	51.17
10	HETATM	2044	01	HOH	53	3.499	6.444	14.452	1.00	50.38
	HETATM	2045	01	HOH	54	18.655	-2.048	25.518	1.00	52.29
	HETATM	2046	01	HOH	55	28.188	-15.195	38.996	1.00	55.22
	HETATM	2047	01	HOH	56	35.275	-10.556	38.061	1.00	57.39
	HETATM	2048	01	HOH	57	37.771	-9.103	34.605	1.00	54.17
15	HETATM	2049	01	HOH	58	31.403	-3.039	17.983	1.00	46.80
	HETATM	2050	01	HOH	59	30.455	-6.352	17.005	1.00	47.05
	HETATM	2051	01	HOH	60	25.985	8.255	0.416	1.00	43.32
	HETATM	2052	01	HOH	61	35.679	0.749	10.462	1.00	42.99
20	HETATM	2053	01	HOH	62	14.741	4.029	33.936	1.00	49.59
	HETATM	2054	01	HOH	63	16.333	2.592	35.952	1.00	45.13
	HETATM	2055	01	HOH	64	23.809	7.186	39.798	1.00	45.36
	HETATM	2056	01	HOH	65	27.012	-1.948	46.995	1.00	63.39
	HETATM	2057	01	HOH	66	25.956	-6.422	42.144	1.00	44.94
	HETATM	2058	01	HOH	67	23.510	-8.414	39.036	1.00	39.06
25	HETATM	2059	01	HOH	68	41.475	0.971	33.110	1.00	55.50
	HETATM	2060	01	HOH	69	36.519	8.863	38.836	1.00	41.56
	HETATM	2061	01	HOH	70	30.111	14.823	12.793	1.00	44.58
	HETATM	2062	01	HOH	71	26.850	-6.092	1.594	1.00	40.15
30	HETATM	2063	01	HOH	72	20.448	-3.169	1.055	1.00	42.50
	HETATM	2064	01	HOH	73	33.896	3.047	16.172	1.00	46.39
	HETATM	2065	01	HOH	74	16.884	0.446	26.043	1.00	61.50
	HETATM	2066	01	HOH	75	18.595	0.296	27.866	1.00	47.33
	HETATM	2067	01	HOH	76	6.166	21.439	19.124	1.00	47.94
	HETATM	2068	01	HOH	77	18.484	20.060	16.232	1.00	35.52
35	HETATM	2069	01	HOH	78	1.985	23.265	29.187	1.00	46.42
	HETATM	2070	01	HOH	79	12.729	30.461	27.530	1.00	62.79
	END									

5 Phe Lys Asn Leu Pro Leu Glu Asp Gln Ile Thr Leu Ile Gln Tyr Ser  
                     20                    25                    30

Trp

10

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Trp

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40 <212> PRT

<213> Homo sapiens

<400> 51

Asp Phe Pro Glu Met Met Ala Glu Ile Ile Ser Val

1

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50

# WHAT IS CLAIMED IS:

55 1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof.

5 screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to said nuclear receptor.

10 2. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.

15 3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

20 4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

25 5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

30 6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

35 7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

8. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5

5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

9. The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

10

10. The method of claim 1, wherein said screening is *in vitro*.

11. The method of claim 10, wherein said screening is high throughput screening.

15

12. The method of claim 1, wherein said assay is a biological assay.

13. The method of claim 1, wherein said test compound is from a library of compounds.

20

14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.

15. The method of claim 14, wherein said test compound is a small organic molecule, a peptide, or peptidomimetic.

25

16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.

17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:

30

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;

modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

35

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

5           18.    A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected  
10   from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

15           19.    The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.

20           20.    The machine readable storage medium of claim 19, wherein said thyroid receptor is human.

          21.    The machine readable storage medium of claim 20, wherein said molecule is peptide.

25           22.    The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.

30           23.    The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

35           24.    A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group

- 5 consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

25. A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.

10

26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.

27. The cocrystal of claim 26, wherein said thyroid receptor is human.

15

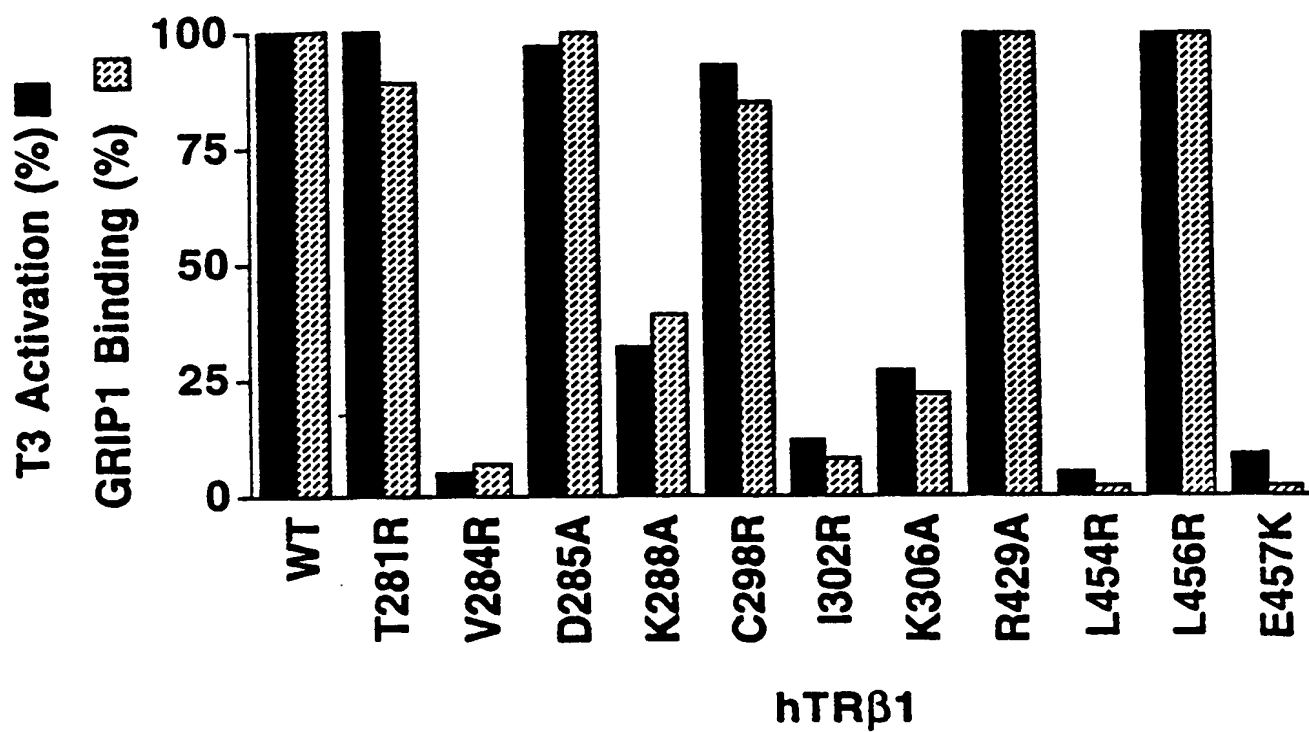
28. The cocrystal of claim 27, wherein said molecule is peptide.

29. The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.

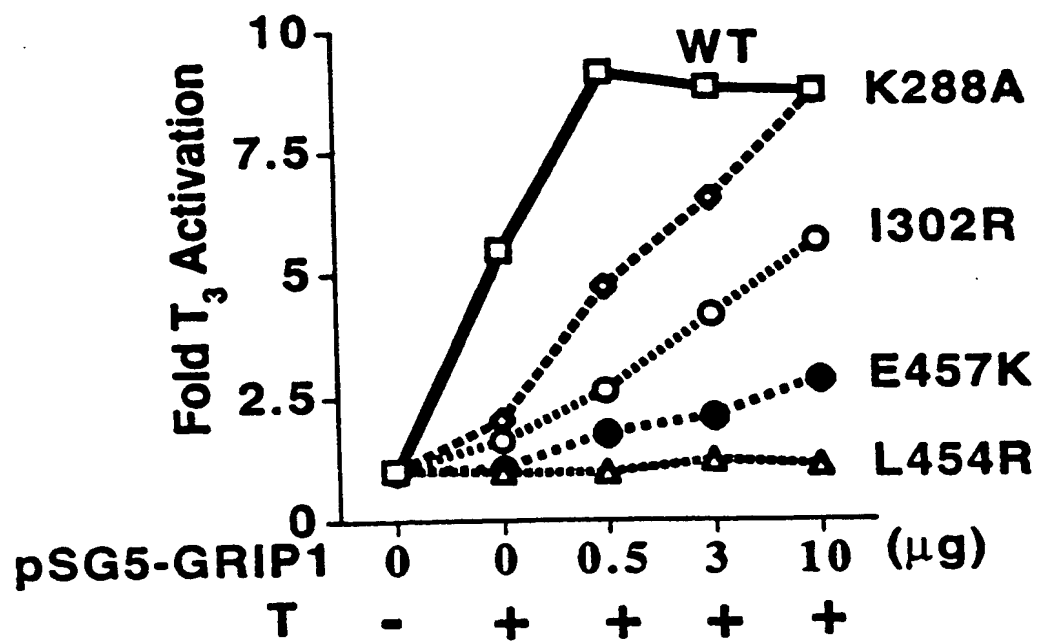
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30. A compound identified according to the method of claim 1.

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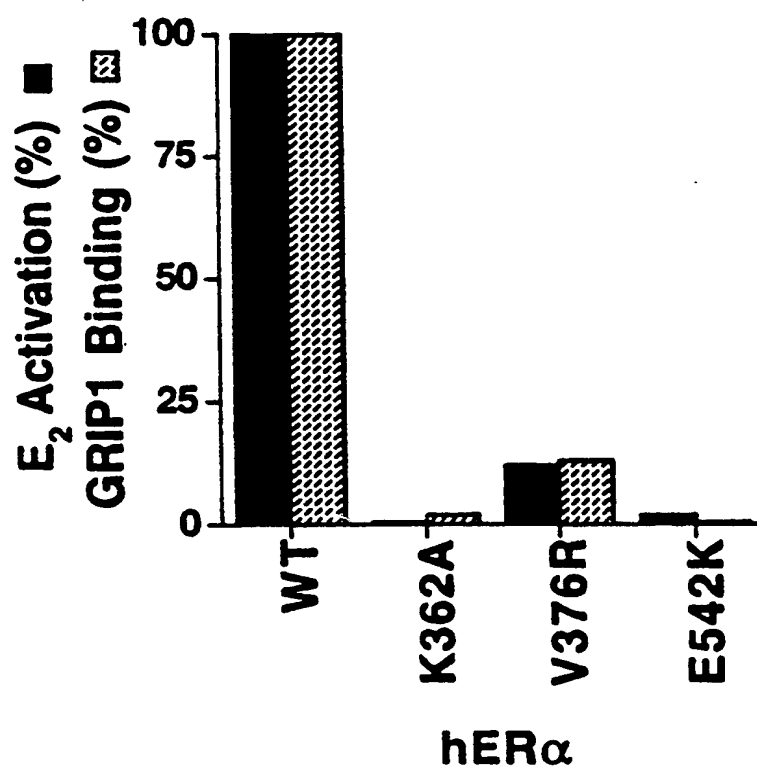
**FIGURE 1**

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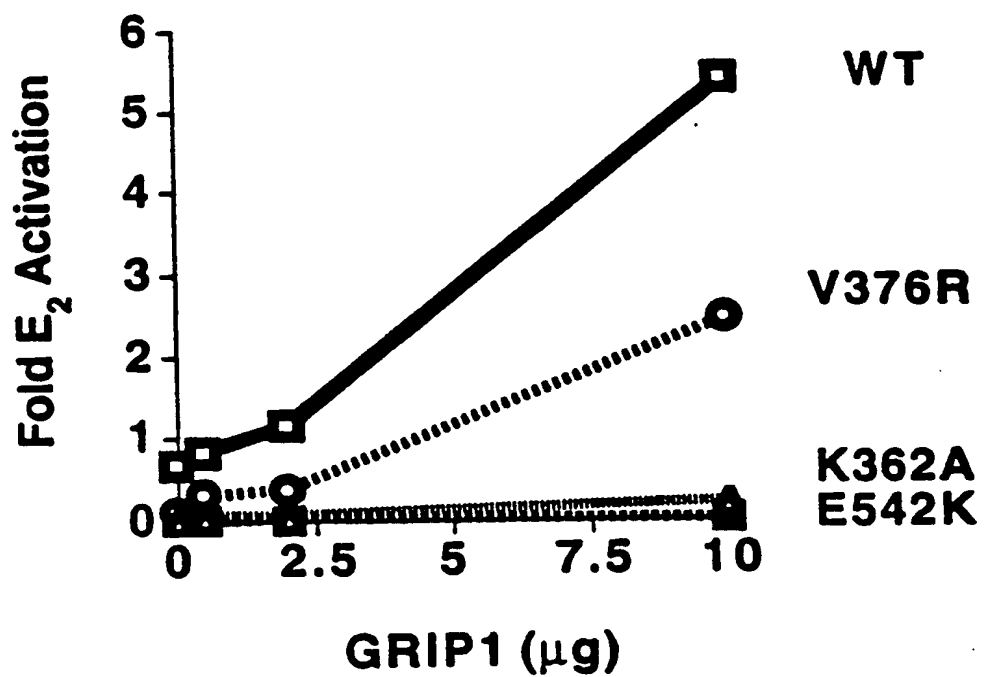
**FIGURE 2**



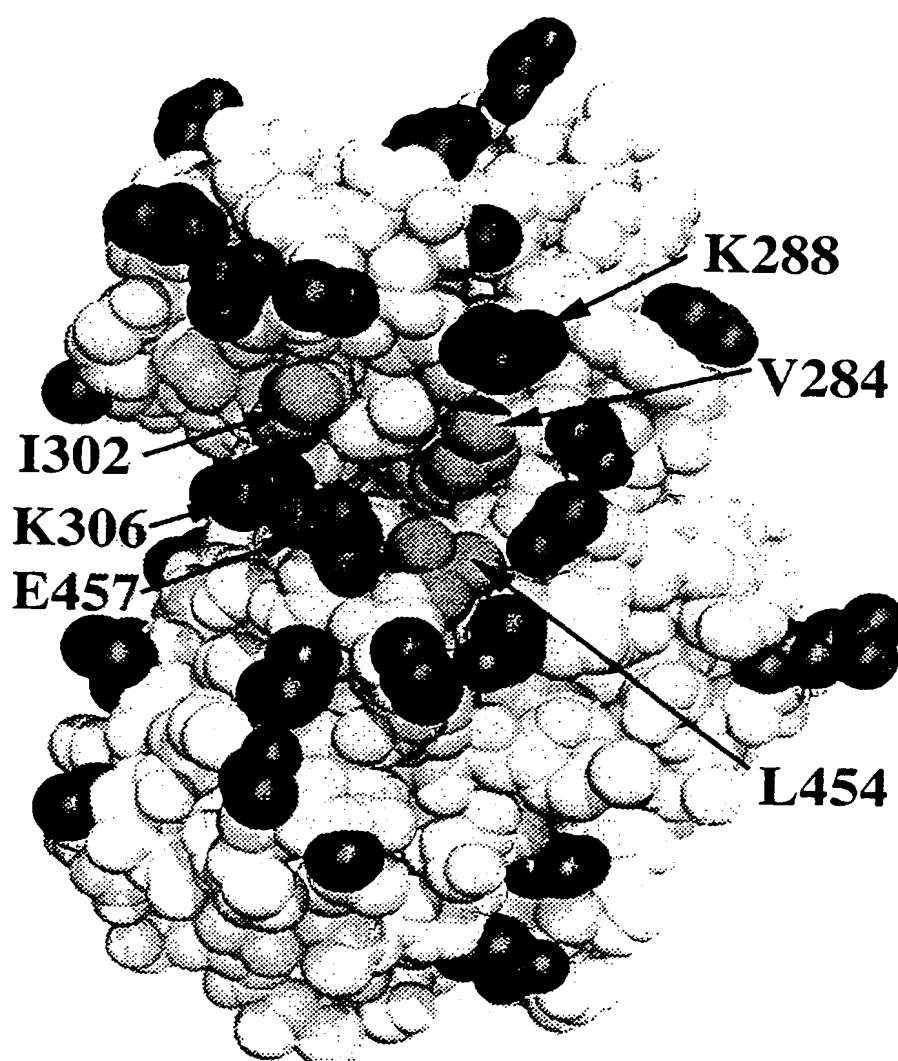
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**FIGURE 3**

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**FIGURE 4**


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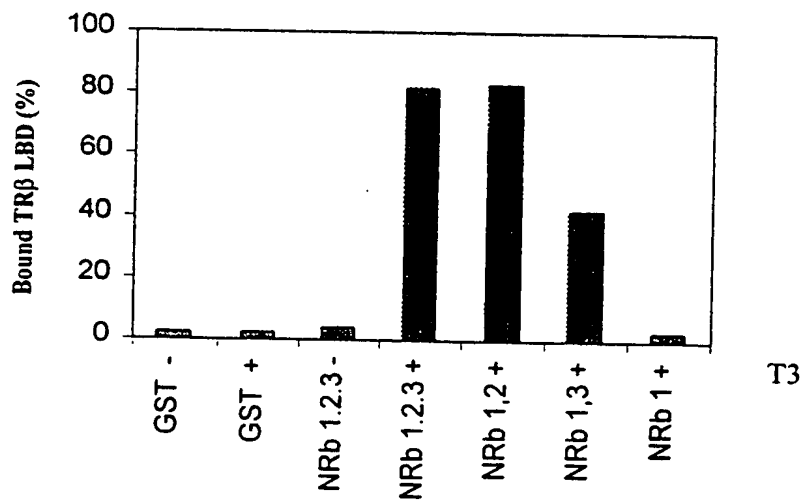
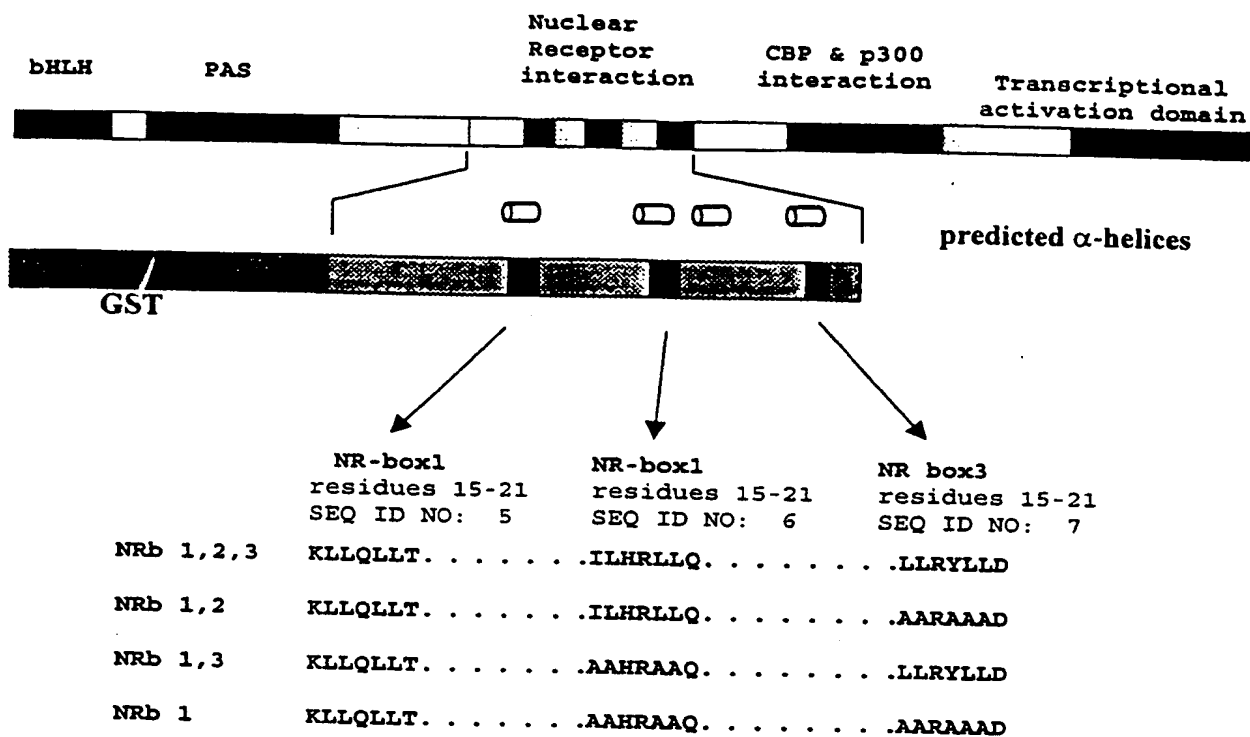
**FIG. 5**

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## FIGURE 6

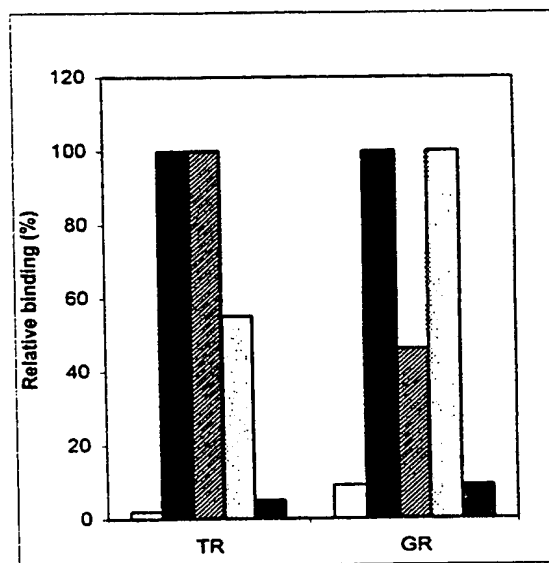
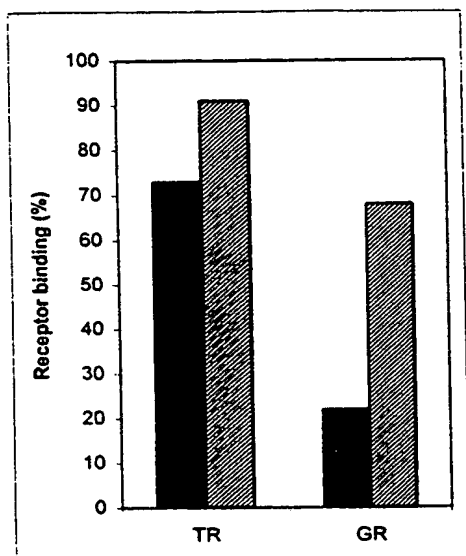
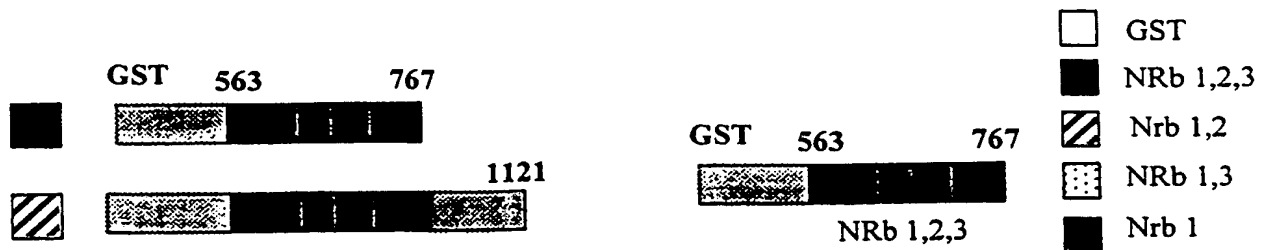
bHLH	PAS	Nuclear Receptor interaction	CBP & p300 interaction	Transcriptional activation domain
				
SEQ ID NO: 5	Grip1	AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS		
SEQ ID NO: 8	Tif2	ADGQSRRLHDSKGQTKLLQLLTTKSEQMEPSPLAS		
SEQ ID NO: 11	NcoA-2	AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLPS		
SEQ ID NO: 14	RAC3	AENQRGPLESKGHKLLQLLTCSSSDRGHSSLTN		
SEQ ID NO: 17	AIB1, TRAM-1	AENQRGPLESKGHKLLQLLTCSSSDRGHSSLTN		
SEQ ID NO: 20	p/CIP	SETPRGPLESKGHKLLQLLTCSSSDRGHSSLTN		
SEQ ID NO: 23	SRC1	SEGDSKY--SQTSHKLVQLLTTTAEQQLRHADID		
SEQ ID NO: 26	Consensus	.....S....KLhQLLT....		
SEQ ID NO: 6	Grip1	PGSTHGTSLSKEKHKILHRLLDSSSPVDLAKLTA		
SEQ ID NO: 9	Tif2	SGSTHGTSLSKEKHKILHRLLDSSSPVDLAKLTA		
SEQ ID NO: 12	NcoA-2	PGSTHGTSLSKEKHKILHRLLDSSSPVDLAKLTA		
SEQ ID NO: 15	RAC3	TSNMHGSLLOEKHRIILHKLQNGNSPAEVAKITA		
SEQ ID NO: 18	AIB1, TRAM-1	TSNMHGSLLOEKHRIILHKLQNGNSPAEVAKITA		
SEQ ID NO: 21	p/CIP	TSNVHGSLLOEKHRIILHKLQNGNSPAEVAKITA		
SEQ ID NO: 24	SRC1	TCPSSHSSSLTERHKILHRLLOE.GSPSDITTLSV		
SEQ ID NO: 27	Consensus	.....L.E+H+ILH+LLQ...SP.-h..h..		
SEQ ID NO: 7	Grip1	EPASPKKKE---NALLRYLLDKDDTKDIGLPEIT		
SEQ ID NO: 10	Tif2	EPVSPKKKE---NALLRYLLDKDDTKDIGLPEIT		
SEQ ID NO: 13	NcoA-2	EPASPKKKE---NALLRYLLDKDDTKDIGLPSIT		
SEQ ID NO: 16	RAC3	EQLSPKKKE--NNALLRYLLDRDDPSDVLAKKLQ		
SEQ ID NO: 19	AIB1, TRAM-1	EQLSPKKKE--NNALLRYLLDRDDPSDALSKELQ		
SEQ ID NO: 22	p/CIP	EQLSPKKKE--NNALLRYLLDRDDPSDALSKELQ		
SEQ ID NO: 25	SRC1	ELDAAKKESKDHQLLRYLLDKDEKDLRSTPNLC		
SEQ ID NO: 28	Consensus	E....KKKE....LLRYLLD+D-.....h.		
Overall Consensus (SEQ ID NO: 1)		.....LXXLL.....		

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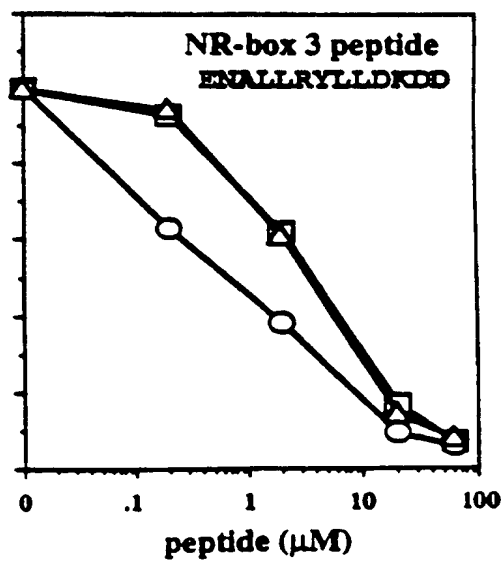
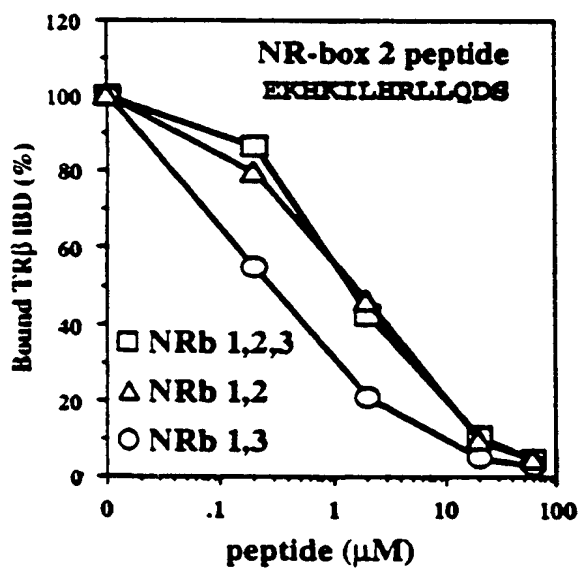
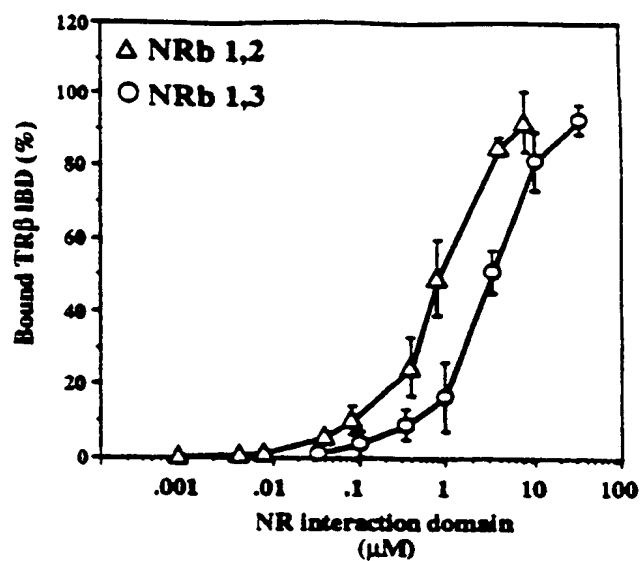
**FIGURE 7**

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# FIGURE 8



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**FIGURE 9**

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## FIGURE 10

residues 11-23  
residues 7-24  
Of  
SEQ ID NO: 6

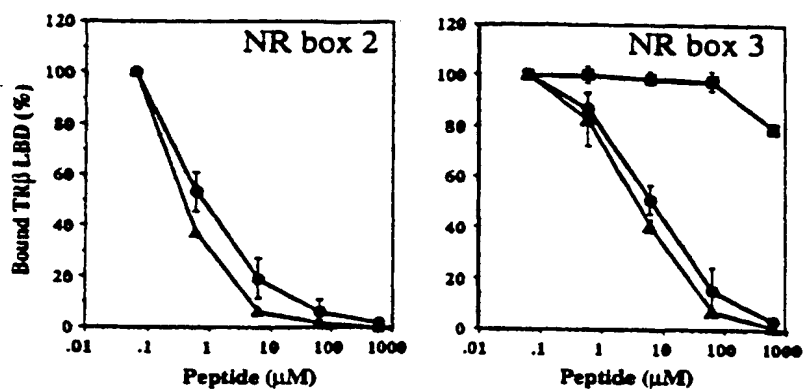
—●—  
—▲—

ETCHK QDS  
TSLKEKHK QDSS

—■—  
—●—  
—▲—

LLRYLL  
KENA LLRYLL DKDDTKD  
PKKKENA LLRYLL DKDDTKD

residues 15-20  
residues 11-27  
residues 8-27  
Of  
SEQ ID NO: 7



residues 8027 of SEQ ID NO: 7  
residues 11-27 of SEQ ID NO: 6  
SEQ ID NO: 29

—▲—  
—▲—  
—▲—

PKKKENA LLRYLL DKDDTKD  
TSLKEKHK QDSS  
TSLKEKHK LLRYLL QDSS

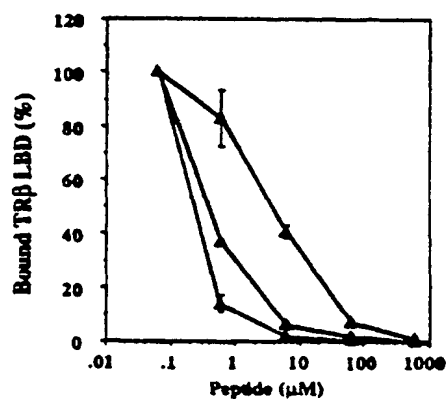
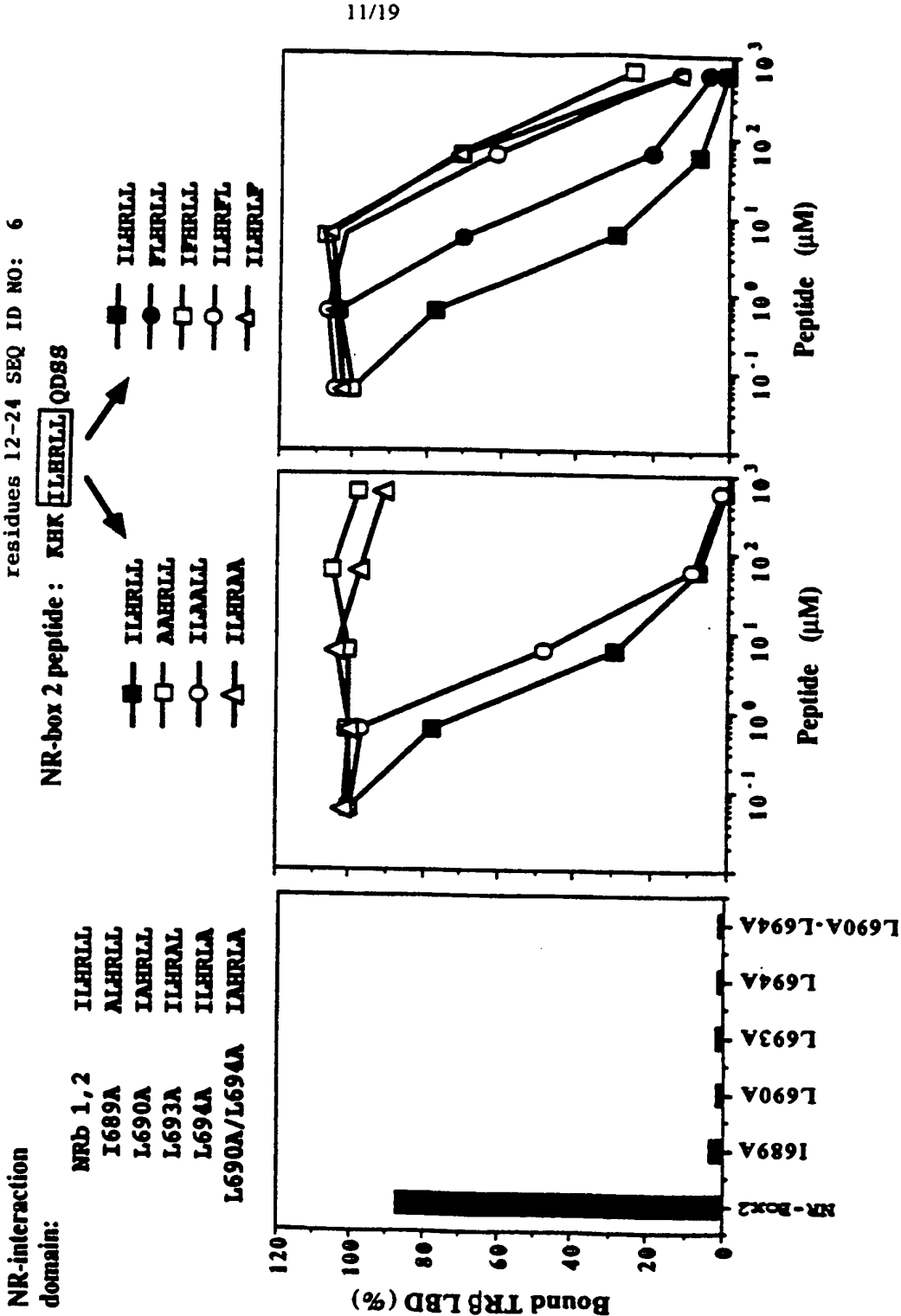
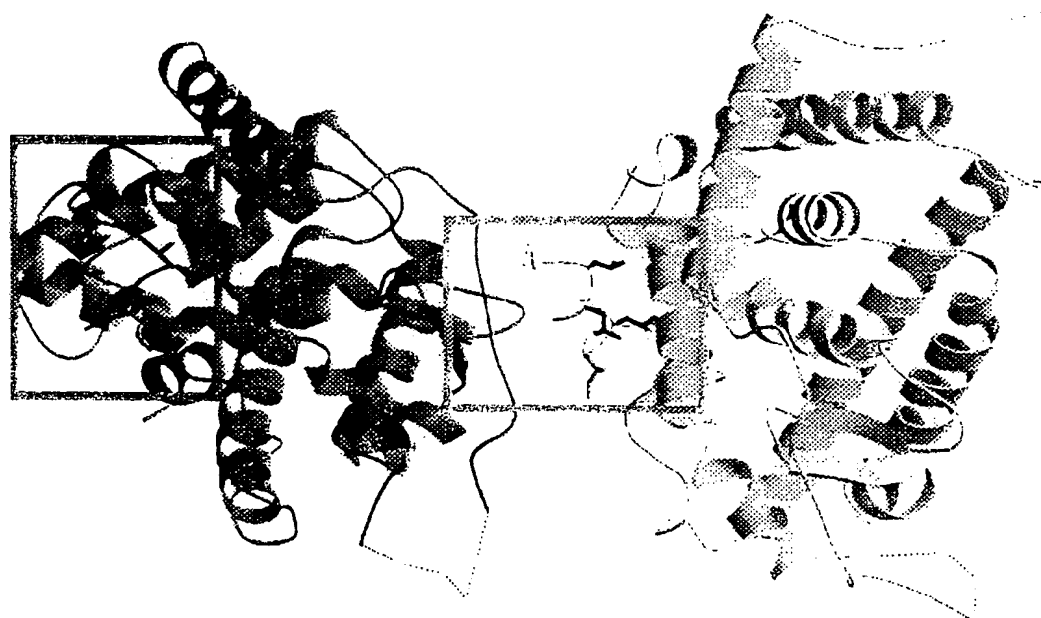




FIGURE 11

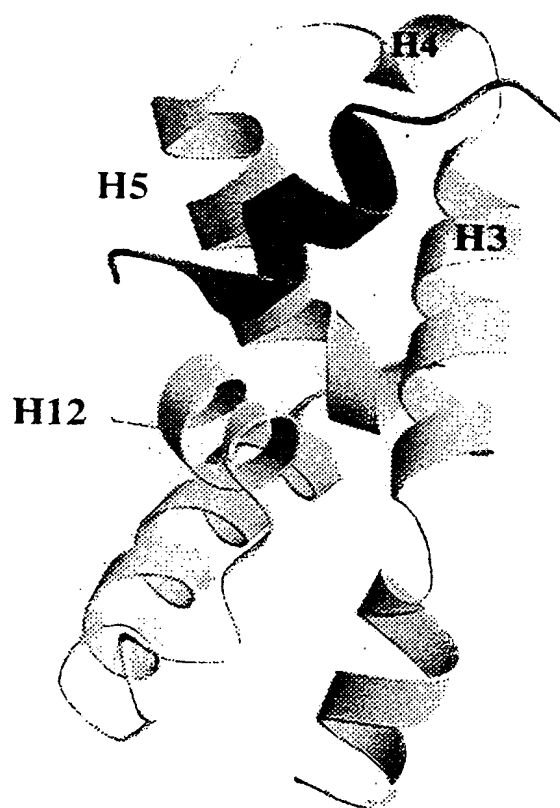


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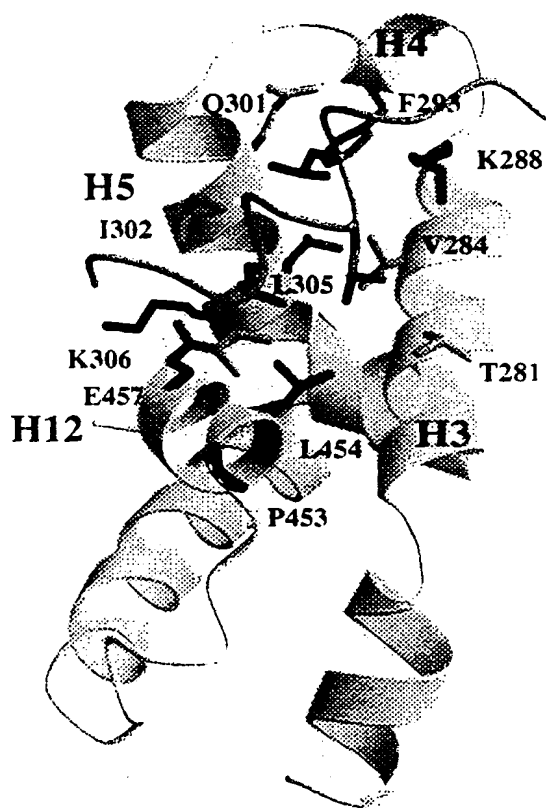
**FIG. 12**

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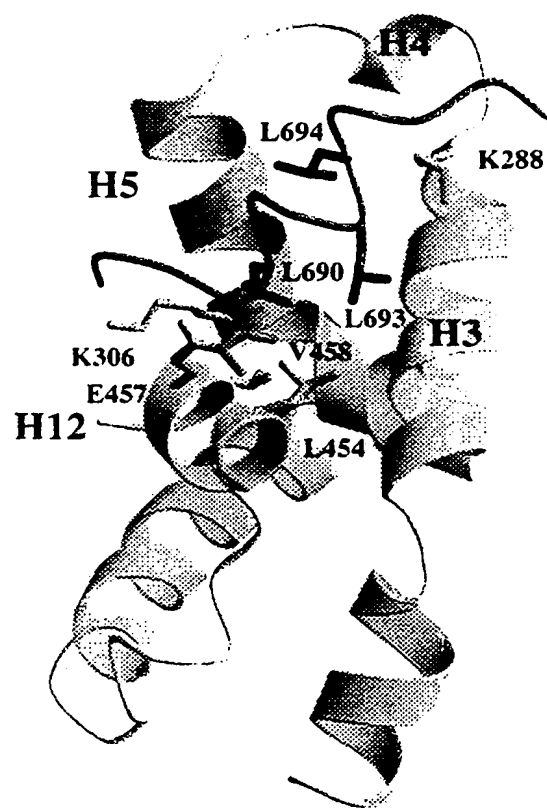
**FIG. 13**

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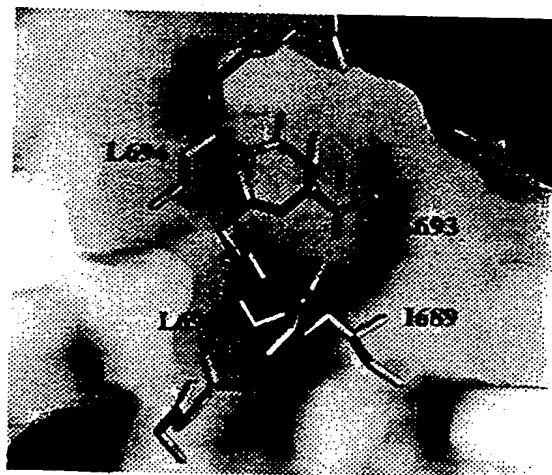
**FIG. 14**

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**FIG. 15**

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**FIG. 16**

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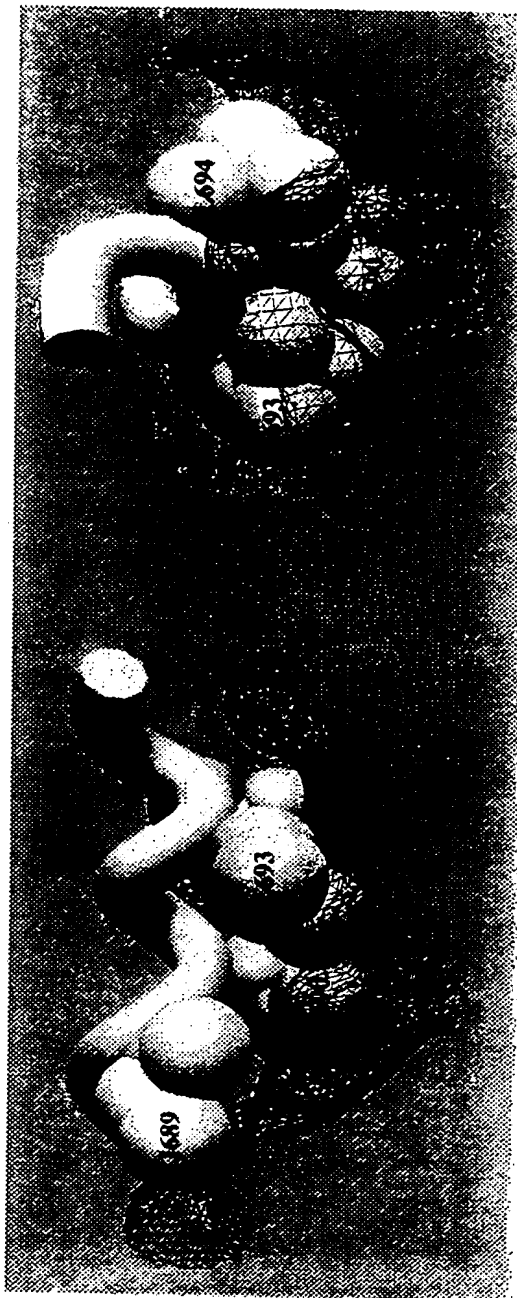
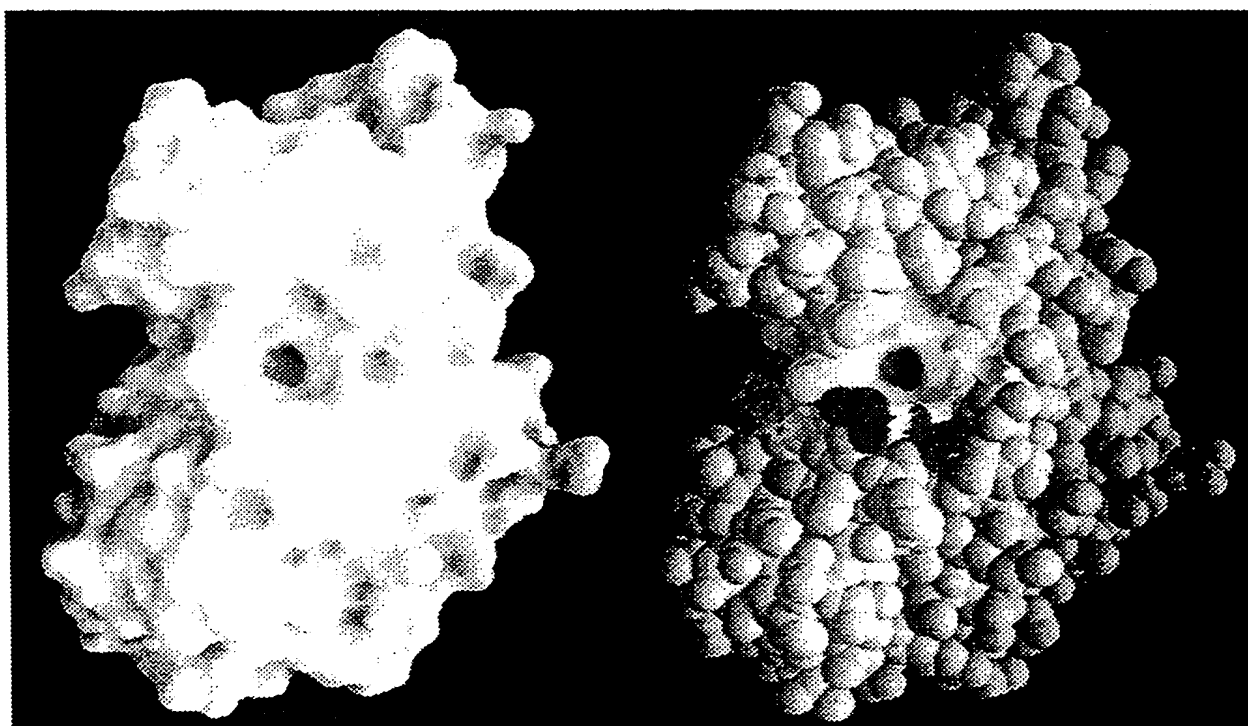


FIG. 17

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**FIG. 18**



## FIGURE 19

## 5 SEQUENCE LISTING

<110> Baxter, John D.  
Darimont, Beatrice  
Feng, Weijun  
10 Fletterick, Robert J.  
Kushner, Peter J.  
Wagner, Richard L.  
West, Brian L.  
Yamamoto, Keith R.

15 <120> METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR  
COACTIVATOR BINDING

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              Leu Gln Leu Leu Thr Thr Lys Ser Glu Gln Met Glu Pro Ser Pro Leu  
                                  20                            25                            30

20            Ala Ser

25            <210> 6  
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30 His Arg Leu Leu Gln Asp Ser Ser Ser Pro Val Asp Leu Ala Lys Leu  
20 25 30

Thr Ala

35

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1 5 10 15

45

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20 25 30

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20 25 30

Ala Ser

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<210> 13  
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10 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Ser Ile Thr  
20 25 30

&lt;210&gt; 14

15 &lt;211&gt; 34

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&lt;213&gt; Homo sapiens

&lt;400&gt; 14

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1 5 10 15

Leu Gln Leu Leu Thr Cys Ser Ser Glu Asp Arg Gly His Ser Ser Leu  
20 25 30

25

Thr Asn

30 &lt;210&gt; 15

&lt;211&gt; 34

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

35 &lt;400&gt; 15

Thr Ser Asn Met His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu  
1 5 10 15

40 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile  
20 25 30

Thr Ala

45

&lt;210&gt; 16

&lt;211&gt; 32

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

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&lt;400&gt; 16

Glu Gln Leu Ser Pro Lys Lys Lys Glu Asn Asn Ala Leu Leu Arg Tyr  
1 5 10 15

55 Leu Leu Asp Arg Asp Asp Pro Ser Asp Val Leu Ala Lys Lys Leu Gln  
20 25 30

60

&lt;210&gt; 17

&lt;211&gt; 34

&lt;212&gt; PRT

65 &lt;213&gt; Homo sapiens

&lt;400&gt; 17

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    1                              5                              10                              15  
    Leu Gln Leu Leu Thr Cys Ser Ser Asp Asp Arg Gly His Ser Ser Leu  
                               20                              25                              30  
 10 Thr Asn

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 25                              20                              25                              30  
    Thr Ala

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35 <400> 19  
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      1                              5                              10                              15  
 40 Leu Leu Asp Arg Asp Asp Pro Ser Asp Ala Leu Ser Lys Glu Leu Gln  
                               20                              25                              30

45 <210> 20  
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 55 Leu Gln Leu Leu Thr Cys Ser Ser Glu Asp Arg Gly His Ser Ser Leu  
                               20                              25                              30  
    Thr Asn

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      <213> Homo sapiens

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 10 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile  
 20 25 30  
 Thr Ala  
 15  
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 25 Leu Leu Asp Arg Asp Asp Pro Ser Asp Ala Leu Ser Lys Glu Leu Gln  
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 60 Val  
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Leu Cys

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                     20                    25                    30

Xaa Xaa

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- Xaa Xaa
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- 55 Arg Tyr Leu Leu Asp Xaa Asp Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa  
                     20                    25                    30
- Xaa Xaa
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 1 5 10 15

Ser Ser

10

<210> 30

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Cys

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35 20 25 30  
Cys

40 <210> 33  
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1 5 10

50 <210> 34  
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Phe Thr Gly Leu Ser Ile Ala Asp Gln Ile Thr Leu Leu Lys Ala Ala  
60 20 25 30  
Cys

65 <210> 35

- 5 <211> 12  
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1 5 10
- 15 <210> 36  
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Phe Ser Glu Leu Pro Leu Asp Asp Gln Val Ile Leu Leu Lys Ala Gly  
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## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

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<b>(54) Title:</b> METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING  <b>(57) Abstract</b> <p>The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.</p>		

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# INTERNATIONAL SEARCH REPORT

International application No.  
PCT/US99/06899

## A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) : G01N 33/50

US CL : 435/7.1

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/7.1

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

Please See Extra Sheet.

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X ----- A	WAGNER et al. A structural role for hormone in the thyroid hormone receptor. Nature. 14 December 1995, Vol. 378, pages 690-697, especially page 690 and figure 1 and 2 and Table 1.	1 ----- 2-30

☐

Further documents are listed in the continuation of Box C.

☐

See patent family annex.

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Date of the actual completion of the international search

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Date of mailing of the international search report

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# INTERNATIONAL SEARCH REPORT

International application No.  
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## Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

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- ☐ The additional search fees were accompanied by the applicant's protest.  
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CORRECTED VERSION

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(74) Agents: HUNTER, Tom et al.; Law Offices of Jonathan Alan Quine P.O. Box 458, Alameda, CA 94501 (US).

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(72) Inventors: BAXTER, John, D.; 131 San Pablo Avenue, San Francisco, CA 94127 (US). DARIMONT, Beatrice; 1441 Tenth Avenue, San Francisco, CA 94122 (US). FENG, Weijun; 105 Johnstone Drive, San Francisco, CA 94131 (US). FLETTERICK, Robert; 15 Christopher Avenue, San Francisco, CA 94131 (US). KUSHNER, Peter, J.; 1362 6th Avenue, San Francisco, CA 94122 (US). WAGNER, Richard, L.; 1701 Waller Street, San Francisco, CA 94117 (US). WEST, Brian, L.; 142 Anderson Street, San Francisco, CA 94110 (US). YAMAMOTO,

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(54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

(57) Abstract: The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

WO 99/060014 A3

## METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

## ACKNOWLEDGEMENTS

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## INTRODUCTION

### Technical Field

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

## Background

Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called “orphan receptors” for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

5 Although overall sequence conservation between nuclear receptors varies between different families  
of receptors, sequence conservation between functional regions, or modules, of the receptors is  
high. For example, nuclear receptors can be organized into functional modules comprising an N-  
terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal  
ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-  
10 dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to  
modulate transcription of DNA, although they may have transcription-independent actions. Nuclear  
receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are  
involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease  
binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear  
15 receptors on transcription. For example, nuclear receptors can stimulate transcription in response to  
hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al.,  
*Curr. Opin. Cell Biol.* (1997) 9:222-32); and Horwitz et al., *Mol. Endocrinol.* (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain,  
called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in  
20 coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.*  
(1997) 94:248-253; VDR: Jurutka et al., *J. Biol. Chem.* (1997) 272:14592-14599, Masayama et al.,  
*Mol. Endocrinol.* (1997) 11:1507-1517; ER and RAR: Henttu et al., *Mol. Cell Biol.* (1997) 17:1832-  
1839). While these studies support the physiological relevance of the observed interaction, the  
structural and functional nature of the site to which coactivators bind has not been defined.

25 The medical importance of nuclear receptors is significant. They have been implicated in  
breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism,  
hypercholesterolemia, obesity and other conditions. However, limited treatments are available and  
current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the  
receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors  
30 are desired for drug development, the structural and functional basis of such sites, including the  
coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding  
sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator  
proteins. This would provide a major new target for iterative drug design, synthesis, and selection.  
35 It also would be advantageous to devise methods and compositions for reducing the time required to  
discover compounds that target the coactivator binding site of nuclear receptors and administer  
them to organisms to modulate physiological processes regulated by nuclear receptors.

## 5 Relevant Literature

Wagner et al., (*Nature* (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., *supra*; O'Donnell et al., *Mol. Endocrinol.* (1991) 5:94-99; Whitfield et al., *Mol. Endocrinol.* (1995) 9:1166-79; Saatcioglu et al., *Mol. Cell Biol.* (1997) 17:4687-95; Collingwood et al., *supra*; Kamei et al., *Cell* (1996) 85:403-14). Hong et al. (*Proc. Natl. Acad. Sci. USA* (1996) 93(10):498-49452) and Hong et al. (*Mol. Cell. Biol.* (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (*Nature* (1997) 387:677-84), Le Douarin et al., (*EMBO J* (1996) 15:6701-6715) and Heery et al. (*Nature* (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

## SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by



- 5 binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by  
10 homology to the coactivator binding site of human TR described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

- 15 Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or  
20 in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator  
25 binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a  
30 machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

- Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by  
35 modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator

5 binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors. The unique features involved in receptor-selective coactivator binding can be identified by  
10 comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

15

### **BRIEF DESCRIPTION OF THE DRAWINGS**

**Figure 1** shows the specific effects of mutations on hTR $\beta$ 1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T<sub>3</sub> dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant.  
20 GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

**Figure 2** shows that overexpression of full-length GRIP1 rescues loss of transcriptional  
25 activation by hTR $\beta$ 1 mutants. Indicated amounts of the expression vector for full-length GRIP1, pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in **Figure 1**. The WT or different representative hTR $\beta$ 1 mutants are indicated.

**Figure 3** shows specific hER $\alpha$  surface mutants cause loss of transcriptional activation in HeLa cells in parallel with their loss of *in vitro* GRIP1 binding. The fold E<sub>2</sub> activation, expressed as  
30 the percentage of WT, and the phosphorimager quantitation of *in vitro* binding of [<sup>35</sup>S]-labeled hER $\alpha$  WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

5       **Figure 4** shows a plot of the fold  $E_2$  activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for **Figure 3**. The WT or different hER $\alpha$  mutants are indicated. The data represent the averages of three independent experiments, with standard deviations less than 10%.

10       **Figure 5** shows a CPK model of the TR $\alpha$ -LBD, indicating the LBD surface locations of mutations made in the full-length hTR $\beta$ 1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1 $\alpha$  binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues,  
15       respectively. The main chain structures of the TR $\alpha$ - and TR $\beta$ -LBDs are the same (data not shown).

**Figure 6** shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

20       **Figure 7** shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TR $\beta$  LBD. Single letter designations are used for the amino acids.

**Figure 8** shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

25       **Figure 9** shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

**Figure 10** shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of  
30       NR-box-TR $\beta$  LBD interactions.

5           **Figure 11** shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TR $\beta$  LBD.

10           **Figure 12** shows the contents of the asymmetric unit of the crystallized hTR $\beta$  LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in  
15 both bound peptides.

**Figure 13** shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTR $\beta$  LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of  $\alpha$ -helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTR $\beta$  LBD, and the neighboring monomer, are omitted for clarity.

20           **Figure 14** shows interface between the GRIP1 NR-box 2 peptide and the hTR $\beta$  LBD. Side chains of residues of the hTR $\beta$  LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID  
25 NO: 2) ILxxLL motif shown explicitly.

**Figure 15** shows residues in the hTR $\beta$  LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTR $\beta$  LBD.

30           **Figure 16** shows molecular surface of the hTR LBD. The side chains of the leucines residues fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

5           **Figure 17** shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucine residues fit into pockets of the coactivator binding site of the hTR $\beta$  LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

10           **Figure 18** shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding  
15 site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

**Figure 19** shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes  
20 represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.

5

**DESCRIPTION OF SPECIFIC EMBODIMENTS**

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear  
10 receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown  
15 structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding  
20 to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a  
25 prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

30 The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR

5 residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER  
10 LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

15 Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor  
20 structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be  
25 identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor  
30 residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site  
35 may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284, Lys288, Ile302, Lys306, Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus,

5 for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

10 The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and  
15 other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

20 Compounds of particular interest fit spacially and preferentially into the coactivator binding site. By "fits spacially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of  
25 hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a  
30 biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

35 The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single



5 gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR:  $\alpha$ ,  $\beta$ ) or three (RAR, RXR, and PPAR:  $\alpha$ ,  $\beta$ ,  $\gamma$ ) genes or have alternate RNA splicing.

10 The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained  
15 structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface  
20 shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in Figure 19). As described in the Examples, the cocrystal of the hTR $\beta$  LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide.  
25 Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO:  
30 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix  
35 motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

5 For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be used to predict how a small molecule of interest can interact with the nuclear receptor coactivator binding site. Fragment-based docking also can be used in building molecules *de novo* inside the coactivator binding site, by placing chemical fragments that complement the site to optimize  
10 intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new  
15 compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

20 Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule  
25 databases include any virtual or physical database, such as electronic and physical compound library databases, and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR),  
30 using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual  
35 inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and

- 5 molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

- 20 Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, *J. Med. Chem.* (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202; available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, *J. Mol. Biol.* (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

- 30 Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

5           Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL  
10 Information Systems, San Leandro, CA; reviewed in Martin, *J. Med. Chem.* (1992) 35:2145-2154); and HOOK (available from Molecular Simulations, Burlington, MA).

          In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally  
15 including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

20           Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., *J. Med. Chem.* (1990) 33:883-894); Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of  
25 which may be used. See, for example, Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, *Structure*, (1994) 2:577-587); and Kuntz et al., *Science*, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

30           Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

          Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity,  
35 such as a biologically based assay. Screening can be *in vitro* and/or *in vivo*. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening

5 preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

10 As an example, *in vitro* binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues  
15 TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein  
20 and in Shibata et al. (*Recent Prog. Horm. Res.* 52:141-164 (1997)); Tagami et al. (*Mol. Cell Biol.* (1997) 17(5):2642-2648); Zhu et al. (*J. Biol. Chem.* (1997) 272(14):9048-9054); Lin et al. (*Mol. Cell Biol.* (1997) 17(10):6131-6138); Kakizawa et al. (*J. Biol. Chem.* (1997) 272(38):23799-23804); and Chang et al. (*Proc. Natl. Acad. Sci. USA* (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments  
25 thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., *MCB supra*; and Hong et al., *PNAS supra*) and/or SRC-1 (Spencer et al., *Nature* (1997) 389:194-198; Onate et al., *Science* (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist  
30 activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric  
35 effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

5 Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to  
10 measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include  
15 TR-based disorders including cardiovascular disease, metabolic disorders, hyperthyroidism, glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples,  
20 TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand T<sub>3</sub>.

Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or  
25 small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

After the three dimensional structure of the cocrystal is determined, the structural  
30 information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful  
35 for solving the structure of those other crystal forms of nuclear receptors. They may also be used to

- 5 solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in **Appendix 1**. This method will provide an accurate structural form for the  
10 unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model  
15 of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular  
20 complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interactive drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of  
25 machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of  
30 the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including  
35 members of the steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors

5 that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR- $\alpha$ , human RAR- $\gamma$ , human RXR- $\alpha$ , human RXR- $\alpha$ , human PPAR- $\alpha$ , human PPAR- $\beta$ , human PPAR- $\gamma$ , human VDR, human ER (as described in Seielstad *et al.*, *Molecular Endocrinol.*, (1995) 9:647-658,  
10 incorporated herein by reference), human GR, human PR, human MR, and human AR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2.  
15 A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong *et al.* (*PNAS supra*; and *MCB supra*), for GRIP1 expression, which reference is herein incorporated by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or  
20 as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most  
25 preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR- $\alpha$  or Glu 202 to Asp 461 of the human TR- $\beta$ .

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass  
30 spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC),  
35 and heparin affinity chromatography.



5 To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound  
10 receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with  
15 at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be  
20 established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction  
25 pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can  
30 assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials  
35 at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute

5 components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the hanging drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., supra. The structure is refined following  
10 standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of  
15 the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

5

**EXAMPLES****Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators****A. Human TR $\beta$  LBD**

Human TR $\beta$  LBD (His6-E202-D461) was expressed and purified as described (Shiau et al.,  
10 *Gene* (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28)  
in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for  
24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl,  
10% glycerol, 25mM  $\beta$ -mercaptoethanol and 0.1mM PMSF as described above. The lysate was  
15 cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in  
the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an  
imidazole gradient (12 - 300 mM). TR $\beta$  LBD containing fractions were loaded in 0.6M ammonium  
sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium  
sulfate gradient [0.6 – 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TR $\beta$  LBD  
were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T<sub>3</sub> (Sigma).  
20 The hydrophobic interaction run was repeated with liganded receptor under the same conditions.  
Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed  
to 20mM Hepes pH7.0, 3mM DTT and 0.1  $\mu$ M T<sub>3</sub> using NAP columns (Pharmacia). For  
crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10  
concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter  
25 bacterial culture.

**B. Human TR mutants**

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded  
oligonucleotides which encode the mutant sequence and which have ends allowing them to be  
ligated as a cassette using pairs of the NsiI, PstI, SstI, AlwNI, ApoI, PflMI, BstXI, BseRI, BsmFI,  
30 PvuII, NspI, SmaI, PmlI, BglII and BsmI restriction sites of the hTR $\beta$ 1 cDNA sequence, or the 3'  
plasmid polylinker Sall, or BamHI restriction sites. The hTR $\beta$ 1 sequences thus mutated were  
subcloned into the pCMX vector encoding the full-length 461 amino acid hTR $\beta$ 1 sequence. Some  
of the mutations of the hTR $\beta$ 1 in the CMX vector and all three mutations of the hER $\alpha$  in the pSG5-  
ER-HEGO vector (Tora et al., *EMBO* (1989) 8:1981) were created using Quick Change Site-

- 5 Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

### C. Human ER $\alpha$ LBD

The human ER $\alpha$ -LBD 297-554 was overexpressed as described previously (Seielstad, et al., *supra*) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained  
10 the sequence Met-Asp-Pro fused to residues 297 to 554 of the hER $\alpha$  (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., *Proc. Natl. Acad. Sci. USA* (1980) 77:5115-5119; Landel, et al., *Mol. Endocrinol.* (1994) 8:1407-1419; Landel, et al., *J. Steroid Biochem. Molec. Biol.* (1997) 63:59-73).

15 To carboxymethylate the solvent-accessible cysteines, the bound hER $\alpha$ -LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., *Steroids* (1996) 61:367-373). Protein was eluted with 3 x 10<sup>-5</sup> M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hER $\alpha$ -LBD was typically close to 100% (Seielstad, et al., *Biochemistry* (1995) 34:12605-12615). The affinity-  
20 purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hER $\alpha$ -LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass  
25 spectrometry.

### D. Human ER mutants

To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ER $\alpha$  LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the  
30 binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind <sup>35</sup>S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

5           <sup>35</sup>S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hER $\alpha$  LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376; 10 L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist, 15 confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

#### E. Human ER LBD-GST Fusion Protein

20           A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hER $\alpha$  was constructed by subcloning the EcoRI fragment from pSG5 ER $\alpha$ -LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were 25 created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

#### F. Radiolabeled full-length receptors and coactivator proteins

30           Wild-type (WT) or mutant pCMV-hTR $\beta$ 1 vector and the pSG5-GRIP1 and pCMX-SRC-1a vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the TNT coupled Reticulocyte Lysate System (Promega) and [<sup>35</sup>S]-Met (DuPont). GST-GRIP1 (amino acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-hTR $\beta$ 1 (full-length, WT or mutants, WT provided by C. Costa), and the GST-hRXR $\alpha$  (full-length

- 5 provided by. C. Costa), fusion proteins were produced in *E. coli* strain HB101 as per the manufacturer's protocol (Pharmacia Biotech).

#### G. Coactivator GRIP1 563-767 His6 GST fusion protein

- GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1 563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I-Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freeze-thawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliquots and stored at -70°C.

#### 30 H. Coactivator GRIP1 563-767 His6

- GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived from pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. The fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl

- 5 pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

### Example 2: Peptide synthesis

- Coactivator peptides were obtained using standard techniques. All peptides were HPLC  
10 purified and analyzed by mass spectroscopy. Peptide concentrations were either determined spectroscopically using the tyrosine signal ( $A_{276} = 1450 \text{ M}^{-1}\text{cm}^{-1}$ ) or by amino acid analysis following standard techniques.

### Example 3: Binding assays with nuclear receptors and coactivators

#### A. GST-GRIP Pull-down Assays and Peptide Competition Assays

- 15 Binding experiments were performed by mixing glutathione beads containing 10  $\mu\text{g}$  of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2  $\mu\text{l}$  of the [ $^{35}\text{S}$ ]-labeled wild-type or mutant hTR $\beta$ 1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150  $\mu\text{l}$  of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM  $\text{MgCl}_2$ , 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the  
20 presence or absence of 1  $\mu\text{M}$   $\text{T}_3$ . Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

- For *in vitro* binding studies GR, TR and their derivatives were translated in the presence of [ $^{35}\text{S}$ ]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were  
25 performed in the presence and absence of 10 $\mu\text{M}$  dexamethasone or 1 $\mu\text{M}$  RU486 for GR and 10 $\mu\text{M}$  triiodothyronine for TR. Expression was quantified by phosphorimager analysis (BAS2000, Fuji). For all binding assays 50 $\mu\text{l}$  of a 20% bead suspension containing either 1.6 or 4.0  $\mu\text{M}$  bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2 $\mu\text{l}$  or 1.4 $\mu\text{l}$  *in vitro* transcribed and translated TR or GR, respectively. Binding was performed in the binding  
30 buffer described above supplemented with 20  $\mu\text{g}/\text{ml}$  BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of

5 receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200 $\mu$ l binding buffer + BSA at 4°C before elution of the bound proteins in 20 $\mu$ l SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was  
10 determined by phosphoimager analysis.

#### B. GST-hTR $\beta$ 1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [ $^{35}$ S]-labeled full-length GRIP1, [ $^{35}$ S]-labeled full-length SRC-1a, and [ $^{35}$ S]-labeled full-length hRXR $\alpha$ , to GST-hTR $\beta$ 1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and  
15 E457K all bound to hRXR $\alpha$  with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [ $^{35}$ S]-Met-labeled full-length hTR $\beta$ 1 WT and mutants (data not shown).

#### 20 C. GST-hER $\alpha$ LBD Pull-down Assays

The wild-type and mutant GST-hER $\alpha$  LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hER $\alpha$  (H222). Cleared extracts containing the GST- hER $\alpha$  LBDs were  
25 incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1  $\mu$ M of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10  $\mu$ l glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40.  $^{35}$ S-labeled GRIP1 was synthesized by *in vitro*  
30 transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hER $\alpha$  LBDs were incubated for 2.5 hours with 2.5  $\mu$ l aliquots of crude translation reaction mixture diluted in 300  $\mu$ l of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40,



- 5 proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound  $^{35}\text{S}$ -GRIP1 was quantitated by fluorography following SDS-PAGE.

#### D. Electrophoretic Mobility Shift Assays

GRIP1, a mouse p160 coactivator, recognizes the ER $\alpha$  LBD in a ligand-dependent manner. The binding of agonists to the ER $\alpha$ LBD promotes recruitment of GRIP1, whereas binding of  
10 antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ER $\alpha$  strongly prefers NR-box 2 (Ding, et al., *Mol. Endocrinol.* (1998) 12:302-13).

An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ER $\alpha$  LBD in the presence of either DES or OHT. Eight microgram  
15 samples of purified hER $\alpha$ -LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10  $\mu\text{l}$  of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

20 In the presence of the NR-box 2 peptide, the migration of the DES-hER $\alpha$ -LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hER $\alpha$ -LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

#### Example: 4 Transfection assays with TR and hER $\alpha$

25 HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5  $\mu\text{g}$  of the reporter p(DR-4)<sub>2</sub>-TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results  
30 (data not shown). Also, 2  $\mu\text{g}$  of the hTR $\beta$ 1 expression vector, pCMX-TR (WT or mutant), and 0.5  $\mu\text{g}$  transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the  $\beta$ -galactosidase gene, were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s),

5 or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., *supra*), and GC cells expressing TR (Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073).

For hER $\alpha$  assays, 5  $\mu$ g of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, et al., *Mol Cell Biol.* (1995) 15:1554), 0.5  $\mu$ g  
 10 expression vector encoding full-length hER $\alpha$ , pSG5-er HEGO (WT or mutants), and 2  $\mu$ g of pj3lacZ, were used. For the experiments of Figures 2 and 4, 0.5  $\mu$ g of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were treated with or without 1  $\mu$ M T<sub>3</sub> or E<sub>2</sub>, as indicated. After culturing for 24 hrs, the LUC or CAT  
 15 activities were assayed and the  $\beta$ -galactosidase activities were also assayed to correct for differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

#### Example 5: Hormone binding assays for wild-type and mutant TRs

The T<sub>3</sub> binding affinity constants (K<sub>d</sub>) for *in vitro* -translated WT and mutant TRs were measured using [<sup>125</sup>I] 3,5,3'-triiodo-L-thyronine ([<sup>125</sup>I]T<sub>3</sub>) in gel filtration binding assays as  
 20 described (Apriletti et al., *Protein Expr. Purif.* (1995) 6:363). Both the K<sub>d</sub> and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81  $\pm$  12 pM. The relative affinity was determined by dividing the WT K<sub>d</sub> by each  
 25 mutant K<sub>d</sub>. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R  
 30 (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

#### Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3,5,3'-triiodo-L-thyronine (T<sub>3</sub>) bind equally well to the coactivator, GRIP1. In all cases, GRIP1 binding was hormone-dependent

5 (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (**Figure 1**). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (**Figure 1**). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators  
10 recognize the same TR surface residues.

#### **Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell**

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells. T<sub>3</sub> increased reporter gene activity 5-fold in cells  
15 expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in **Figure 1**). By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to T<sub>3</sub> which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of  
20 GRIP1 binding and activation (**Figure 2**). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

#### **Example 8: Effect of TR mutations on other receptor functions**

The effects of the mutations on other receptor functions also were examined. All of the  
25 mutants bound radiolabeled thyroid hormone (K<sub>d</sub> values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region  
30 spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., *supra*; Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of T<sub>3</sub>-dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al., *supra*), suggesting  
35 that the CBS residues do not participate in TR actions mediated through these proteins. These data

- 5 indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

#### Example 9: Coactivator binding site in ER

- Three separate mutations (K362A, V376R, and E542K) were created in human estrogen  
10 receptor- $\alpha$  (hER $\alpha$ ) which align to three of the effective positions in hTR $\beta$ 1 (K288A, I302R, and E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which  
15 responds to the ER amino-terminal activation function (Berry et al., *EMBO J* (1990) 9:2811-2818) (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

#### Example 10: Coactivator NR-box binding affinity for TR

- 20 To study the interaction between nuclear receptors and GRIP1 *in vitro*, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using Ph.D., displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are  
25 part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

- Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTR $\beta$  LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50 ) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine  
30 does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = 1.0  $\mu$ M) over NR-box 3 (EC50 = 4.0  $\mu$ M) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR.

- 5 Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

**Example 11: Coactivator NR-box binding affinity for GR**

GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (Figure 8). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR  
10 about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial antagonist RU486. These results are in agreement with *in vivo* 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the  
15 absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR  
20 prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

**Example 12: Coactivator peptide binding affinity for TR**

To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or  
25 structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTR $\beta$  LBD were performed using coactivator peptides containing different NR- boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLQLDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (Figure 9). Consistent with the interaction of hTR LBD $\beta$  with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of  
30 GRIP1 with hTR $\beta$  LBD only at very high concentrations ( $EC_{50}$  = 130  $\mu$ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTR $\beta$  LBD for NR-box 2 ( $EC_{50}$  (NR-box 2) = 1.5  $\mu$ M,  $EC_{50}$  (NR-box 3) = 4  $\mu$ M). The apparent affinities ( $EC_{50}$ ) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the  
35 sequence and independent of the structural context of the NR-boxes.

- 5           Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes, TR preferentially binds NR-box 2.

These results show the preference of TR for NR-box 2 is sequence dependent.

- 10           The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

### **Example 13: Binding affinity of TR for extended coactivator peptides**

- Sequence identity between all three central NR-boxes of the p160 coactivator family is  
 15   limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (**Figure 6**). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTR $\beta$  LBD  
 20   were compared (**Figure 10**).

- A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to  
 25   include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the  
 30   context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adjacent sequences.

## 5    **Example 14: Binding affinity of TR and GR for mutant coactivator**

### **A.    TR affinity for ILxxLL motif residues**

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (**Figure 11**). Surprisingly, replacement of  
10    any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTR $\beta$  LBD, it appears that their contribution to the affinity of NR-box 2 for hTR $\beta$  LBD is cooperative rather than additive.

15        Similar results were obtained by competing the interaction of hTR $\beta$  LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (**Figure 11**). Whereas the peptides containing the IL or LL replacement failed to interact with the hTR $\beta$  LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal  
20    effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (**Figure 11**). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues  
25    themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTR $\beta$  LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767)  
30    with hTR $\beta$  LBD.

### **B.    TR affinity of FxxLW and FxxAL motif residues**

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTR $\beta$  LBD:NR-box 2 interaction surface, whereas the non conserved

5 isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTR $\beta$  LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-  
10 KHKILHRLQLDSS-698 is highly complementary to the corresponding binding site in the hTR $\beta$  LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., *Nat Struct Biol.* (1996) 3:87-94; Wagner et al., *supra*; Renaud et al., *Nature* (1995) 378:681-689; Bourguet et al., *Nature* (1995) 375:377-382; and Brzozowski et al., *Nature* (1997) 389:753-758).  
15

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic  $\alpha$ -helices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL)  
20 differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally  
25 interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts  
30 with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very  
35 high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a



- 5 GRIP1 mutant lacking NR-box 3, binds GR *in vivo* (Ding et al., *supra*). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the peptide rather than a particular strong interaction of GR with GRIP1 (563-767).  
10

These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

### C. TR affinity for residues adjacent to ILxxLL motif

- 15 Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (Figure 11). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.  
20

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.  
25

## Example 15: Crystallization and Structure Determination of NR LBD Complexes

### A. Crystallization of hTR $\beta$ LBD with T<sub>3</sub> and GRIP1 NR-box 2 Peptide

- Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the hTR $\beta$  LBD. The complex of the hTR $\beta$  LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTR $\beta$  LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding  
30

5 of prepared drops with microcrystals of the hTR $\beta$  LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTR $\beta$  LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTR $\beta$  LBD determined previously (Wagner et al., *supra*), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTR $\beta$  LBD, residues K211-P254 and G261-D461 of monomer 2  
10 of the hTR $\beta$  LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-KILHRLLQDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLLQD-696 (Appendix 1).

Briefly, the complex between the hTR $\beta$  LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal)  
15 volumes of a solution of 9mg/ml hTR $\beta$  LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTR $\beta$  LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M  
20 ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10<sup>-3</sup> to 10<sup>-5</sup> dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTR $\beta$  LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6).

5

**Table 1**  
**Data collection, phasing, and refinement statistics**

Data collection						
Data set	Resolution (Å)		Reflections		Coverage (%)	R <sub>sym</sub>
Native	3.6		measured	unique	96.3	0.007
			35565	8490		
Rotation search						
Search model	Euler angles (°)				Correlation coefficient	
		Θ <sub>1</sub>	Θ <sub>2</sub>	Θ <sub>3</sub>	Highest peak	Highest false peak
	hTR β LBD	M1	60.12	80.68	241.90	16.3
	M2	9.93	87.70	180.6	15.9	14.2
Translation search						
		Fractional coordinates			Translation function	
		x	y	z	Highest peak (o)	Highest false peak (o)
	M1	0.522	0.428	0.250	19.52	10.02
	M2	0.200	0.932	0.119	26.11	5.77
Refinement						
	Resolution (Å)		Reflection		R	R <sub>free</sub>
F > 2(	25 - 3.7		7614		0.2990	0.3219
All data	25 - 3.7		7851		0.3010	0.317

$R_{\text{sym}} = \sum_h \sum_i |I_{h,i} - \bar{I}_h| / \sum_h \bar{I}_h$  for the intensity ( $I$ ) of  $i$  observations of reflection  $h$ .

Correlation coefficient =  $\sum_h E_o^2 E_c^2 - E_o^2 E_c^2 / [\sum_h (E_o^2 - E_o^2)^2 \sum_h (E_c^2 - E_c^2)^2]^{1/2}$

Translation function ( $t_a, t_b, \dots$ ) =  $\sum_h (|E_o(t_h)|^2 - \sum_h \langle |E_o(t_h)|^2 \rangle) (E_c(t_h, t_a, t_b, \dots))^2 - \langle |E_c(t_h)|^2 \rangle$   
 where  $E_o$  represents the normalized observed structure factor amplitudes, and  $E_c$  represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation ( $t_a, t_b$ ) of the NCS monomers, divided by the rms value of the translation function density.

R factor =  $\sum |F_{\text{obs}} - F_{\text{calc}}| / \sum |F_{\text{obs}}|$ .

$R_{\text{free}}$  is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

5            **B.     Crystallization of hER $\alpha$  LBD with DES and GRIP1 NR-box 2 Peptide**

Crystals of a DES-hER $\alpha$  LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hER $\alpha$  LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two  $\mu$ L samples of this solution were mixed  
10 with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800  $\mu$ L of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2<sub>1</sub> with cell dimensions a=54.09, b=82.22, c=58.04 and  $\beta$ =111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200  
15  $\mu$ m x 40  $\mu$ m x 40  $\mu$ m crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10  $\mu$ M peptide and frozen in an N<sub>2</sub> stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were  
20 processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *Methods Enzymol.* (1997) 276:307-326) using the default -3 $\sigma$  cutoff.

**C.     Crystallization of hER $\alpha$  LBD with OHT**

Crystals of the hER $\alpha$  LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2  $\mu$ L) of a solution containing 3.9  
25 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800  $\mu$ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6<sub>5</sub>22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit  
30 consists of a single hER $\alpha$  LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400  $\mu$ m x 250  $\mu$ m x 40  $\mu$ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N<sub>2</sub> suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a

- 5 wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *supra*) using the default  $-3\sigma$  cutoff.

### Example 16: Structure determination and refinement of NR LBD complexes

#### A. Structure of hTR $\beta$ LBD with T<sub>3</sub> and GRIP1 NR-box 2 Peptide

- Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA  
10 with a 0.3mM collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In *Macromolecular Crystallography, Part A* (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in  
15 AMORE from a model of hTR $\beta$  LBD with the ligand, T<sub>3</sub>, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTR $\beta$  LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTR $\beta$  LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and  
20 conventional difference Fourier maps for the iodine atoms of the T<sub>3</sub> ligand confirmed the correctness of the solution. The iodine atoms for both T<sub>3</sub> ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTR $\beta$  LBD. The electron density could be modeled as a short  $\alpha$ -helix, and the observed side chain  
25 density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTR $\beta$  LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTR $\beta$  LBD:GRP1 site 2 peptide complex are attached as  
Appendix 1.

#### 30 B. Structure of hER $\alpha$ LBD with DES and GRIP1 NR-box 2 Peptide

Initial efforts to determine the structure of the DES-hER $\alpha$  LBD-NR box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4

5 suite: programs for protein crystallography", *Acta Crystallogr.* (1994) D50:760-763) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RAR $\gamma$  LBD (Renaud, et al., *supra*) as the search probe (R=58.2%, CC=35.6% after placement of both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7 Å between  
10 this model and the final model based on C $\alpha$  positions) and incomplete (accounting for only ~45% of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., *Bull. Soc. Chim. Belg.* (1988) 97:655-667) and model refinement in REFMAC (Murshudov, et al., *Acta Crystallogr.* (1997) D53:240-255) (using tight  
15 NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 *Am. Cryst. Assoc. Mtg. Abstr.* (1990) 18:73) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of  
20 weights.

However, although the DES-hER $\alpha$  LBD-NR complex model accounted for ~90% of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The high-resolution data set of the DES-hER $\alpha$  LBD-NR-box 2 peptide complex became available when the  $R_{\text{free}}$  of the OHT-hER $\alpha$  LBD model was ~31%. Both monomers in the asymmetric unit of  
25 the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hER $\alpha$  LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the  
30 simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximum-likelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The  $R_{\text{free}}$  set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03 Å (with no  $\sigma$  cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of  
35 peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hER $\alpha$

- 5 LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% ( $R_{\text{free}}=25.0\%$ ) using data to 2.03 Å resolution.

Ile 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The  $\gamma$ -carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 10 377, the  $\gamma$ -carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ER $\alpha$  LBD (Eng, et al., *Mol. Cell. Biol.* (1997) 17:4644-4653); Lazennec, et al., *Mol. Endocrinol.* (1997) 11:1375-86; White, et al., *EMBO J.* (1997) 16:1427-35). Atomic coordinates of 15 DES-LBD-peptide complex are attached as **Appendix 2**.

5

Table 2

## Summary of Crystallographic Statistics

		<u>Ligand</u>	
<u>Data Collection</u>		<u>DES</u>	<u>OHT</u>
	Space group	P2 <sub>1</sub>	P6 <sub>5</sub> 22
10	Resolution	2.03	1.90
	Observations	104189	269253
	Unique	30265	23064
	Completeness (%)	98.4	99.1
	R <sub>sym</sub> (%) <sup>a</sup>	7.8	7.0
15	Average I/σI	9.8	16.1
<u>Refinement</u>			
	Number of non-hydrogen atoms	4180	2070
	R <sub>cryst</sub> (%) <sup>b</sup> /R <sub>free</sub> (%)	19.9/25.0	23.0/26.1
20	Bond r.m.s. deviation (Å)	0.006	0.006
	Angle r.m.s. deviation (°)	1.05	1.05
	Average B factor (Å <sup>2</sup> )	34.0	40.4
	<sup>a</sup> $R_{\text{sym}} = \sum_i  I_i - \langle I_i \rangle  / \sum_i I_i$ where $\langle I_i \rangle$ is the average intensity over symmetry equivalents		
25	<sup>b</sup> $R_{\text{cryst}} = \sum  F_o - F_c  / \sum  F_o $		

C. Structure of hERα LBD-OHT complex

The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERα LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6<sub>1</sub>22 and P6<sub>5</sub>22. A translation search in P6<sub>5</sub>22 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hERα LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR



5 (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., *Proc. Natl. Acad. Sci. USA* (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the  $R_{\text{free}}$  set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no  $\sigma$  cutoff) were included. The final model consisted of residues 306-  
 10 551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hER $\alpha$  LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% ( $R_{\text{free}}$ =26.2%). Atomic coordinates of OHT-hER $\alpha$  LBD complex are attached as **Appendix 3**.

## 15 **Example 17: Structural analysis of hTR $\beta$ LBD:GRIP 1 NR-box 2 peptide complex**

### **A. Structure of cocrystal complex (contents of asu)**

The asymmetric unit (asu) of the crystal contains two monomers of the hTR $\beta$  LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (**Figure 12**). The structure  
 20 of the hTR $\beta$  LBD, which closely resembles that of the rTR $\alpha$  LBD (Wagner et al., *supra*), consists of twelve alpha-helices and two  $\beta$ -strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTR $\beta$  LBD and the rTR $\alpha$  LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic  $\alpha$ -helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

25 The relation of the two monomers of the hTR $\beta$  LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., *supra*; Brzozowski et al., *supra*). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the  
 30 alpha-helix of the cocrystal peptide contacts monomer 1 of the hTR $\beta$  LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

5           The common interface between both cocrystal peptides and the hTR $\beta$  LBD buries the hydrophobic residues that define the cocrystal peptide (SEQ ID NO: 1) LxxLL sequence motif, residues Ile689, Leu690, Leu693, and Leu694; against the surface of the receptor LBD (Figures 16 and 17). The presence of the second peptide in the crystal, duplicating the interactions of the hydrophobic residues, suggests those interactions are specific and drive the interaction of the peptide with the hTR $\beta$  LBD, while the hydrophilic interactions provide a fortuitous crystal contact and account for the dependence of crystallization on the presence and concentration of the peptide.

#### B.     Structure of the GRIP1 NR-box 2 peptide

15           The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLQLDSS-698). For the NR-box 2 peptide in monomer 1 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., *Science* (1996) 274:948-953), VP16:TAF31 (Uesugi et al., *Science* (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan et al., *Cell* (1997) 91:741-752).

#### C.     Structure of the hTR $\beta$ LBD:GRIP1 NR-box 2 peptide interface

30           The hTR $\beta$  LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are I280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

          The GRIP1 NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but

5 defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue  
10 L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTR $\beta$  LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

#### Example 18: Overall Structure of the DES-hER $\alpha$ -LBD-NR-box 2 Peptide Complex

15 The asymmetric unit of the DES-hER $\alpha$  LBD-NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E<sub>2</sub> and RAL (Brzozowski, et al., *supra* and Tanenbaum, et al., *supra*). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar  
20 structures (r.m.s.d. 0.47 Å based on C $\alpha$  positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E<sub>2</sub> (Brzozowski, et al., *supra*); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic  
25 cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic  $\alpha$  helix.  
30 Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

#### Example 19: Structure of the OHT-hER $\alpha$ LBD Complex

The binding of OHT induces a conformation of the hER $\alpha$  LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES

5 complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket  
10 as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., *supra*).

### Example 20: Coactivator binding site structure and function

#### 15 A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the  
20 design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., **Figures 5, 14, and 15**). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that  
25 NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453,  
30 L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational  
35 change upon hormone binding included Leu454 and Glu457. Thus, the site identified by

5 mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site  
 10 are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19).

The coactivator binding site of TR contains charged and hydrophobic residues at its  
 15 periphery, but only hydrophobic residues at its center (see, e.g., Figures 5 and 18). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (Figure 18), right). Residues contained in helices 3, 5 and 6 (Figure 18, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of  
 20 the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (Figure 18, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in  
 25 the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

#### B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER $\alpha$  LBD buries 1000 Å<sup>2</sup> of predominantly hydrophobic surface area from both  
 30 molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization  
 35 of the binding site of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER $\alpha$  LBD, which is the same NR-box 2 peptide utilized to crystallize the T<sub>3</sub>-TR

5 LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter. These residues are highly conserved among the nuclear receptor super family (Figure 19). Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of exploiting the slight differences among the coactivator binding sites of nuclear receptors in  
10 designing and identifying compounds that target specific nuclear receptors.

The ER $\alpha$  LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-KHKILHRLQLDSS-698 (residues 12-24 of SEQ ID NO: 6)  $\alpha$  helix formed by the side chains of Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with  
15 the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689 and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile 689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The  
20 side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix project away from the ER $\alpha$  receptor and either interact predominantly with solvent or form symmetry contacts. None of the side chains of the polar and charged residues outside the helical region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is  
25 involved in hydrogen bonds or salt bridges with its associated ER $\alpha$  LBD monomer. The  $\epsilon$ -amino group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-terminal three residues of peptide B are displaced from monomer B and interact extensively with a symmetry-related ER $\alpha$  LBD.

30 In addition to interacting with the hydrophobic face of the peptide helix, the ER $\alpha$  LBD stabilizes the main chain conformation of the NR box peptide by forming capping interactions with both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These  
35 interactions position the stabilizing charges of the  $\gamma$ -carboxylate of Glu 542 and  $\epsilon$ -amino group of Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542

- 5 hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the  $\epsilon$ -amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

- 10 Except for the orientation of helix 12, the structure of the peptide binding groove of the ER $\alpha$  LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

- 15 Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) LLEML instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

- 25 Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions. Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its  $\epsilon$ -amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu 380. The Glu 380  $\gamma$ -carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

- 35 In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER $\alpha$  LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the

- 5 OHT complex buries more solvent accessible surface area ( $\sim 1200 \text{ \AA}^2$ ) than the NR box peptide in the DES-ER $\alpha$  LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples  
10 showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator  
15 proteins to nuclear receptors for all members of the nuclear receptor super family.

### REFERENCES

1. U.S. Patent No. 5,331,573
2. U.S. Patent No. 5,500,807
- 20 3. Adams, P. D., Pannu, N. S., Read, R. J., and Brunger, A. T. (1997). *Proc. Natl. Acad. Sci. USA* 94, 5018-23.
4. Apriletti et al., *Protein Expr. Purif.* (1995) 6:363
5. Bartlett et al., In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196
- 25 6. Berry, M., Metzger, D., and Chambon, P. (1990). *EMBO J* 9, 2811-8.
7. Bohm, J. *Comp. Aid. Molec. Design* (1992) 6:61-78
8. Bourguet, W., Ruff, M., Chambon, P., Gronemeyer, H., and Moras, D. (1995). *Nature* 375, 377-82.
9. Brzozowski, A., Pike, A., Dauter, Z., Hubbard, R., Bonn, T., Engstrom, O., Ohman, L., Greene, G., Gustafsson, J., and Carlquist, M. (1997). *Nature* 389, 753-758.
- 30 10. Chang et al., *Proc. Natl. Acad. Sci. USA* (1997) 94(17):9040-9045
11. Cohen et al., *J. Med. Chem.* (1990) 33:883-894
12. Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253
13. DesJalais et al., *J. Med. Chem.* (1988) 31:722-729



- 5 14. Ding, S., Anderson, C., Ma, H., Hong, H., Uht, R., Kushner, P., and Stallcup, M. (1998). *Mol. Endocrinol.* 12, 302-313.
15. Eng, F. C. S., Lee, H. S., Ferrara, J., Willson, T. M., and White, J. H. (1997). *Mol. Cell. Biol.* 17, 4644-4653.
16. Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980)
- 10 17. Furey, et al., PA33 *Am. Cryst. Assoc. Mtg. Abstr.* (1990) 18:73
18. Glass, C. K., Rose, D. W., and Rosenfeld, M. G. (1997). Nuclear receptor coactivators. *Curr. Opin. Cell Biol.* 9, 222-32.
19. Goodford, *J. Med. Chem.* (1985) 28:849-857
20. Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202
- 15 21. Greene, G., Harris, K., Bova, R., Kinders, R., Moore, B., and Nolan, C. (1988). *Mol. Endocrinol.* 2, 714-726.
22. Greene, G., Nolan, C., Engler, J., and Jensen, E. (1980). *Proc. Natl. Acad. Sci. USA* 77, 5115-5119.
23. Heery, D., Kalkhoven, E., Hoare, S., and Parker, M. (1997). *Nature* 387, 733-736.
- 20 24. Hegy, G., Shackleton, C., Carlquist, M., Bonn, T., Engstrom, O., Sjöholm, P., and Witkowska, H. (1996). *Steroids* 61, 367-373.
25. Henttu, P. M., Kalkhoven, E., and Parker, M. G. (1997). *Mol. Cell. Biol.* 17, 1832-9.
26. Hong et al., *Mol. Cell Biol.* (1997) 17:2735-44
27. Hong, H., Kohli, K., Trivedi, A., Johnson, D. L., and Stallcup, M. R. (1996). *Proc. Natl. Acad. Sci. USA* 93, 4948-4952.
28. Horwitz et al., *Mol. Endocrinol.* (1996) 10:1167-77
29. Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976
30. Jurutka et al., *J. Biol. Chem.* (1997) 272:14592-14599
31. Kakizawa et al., *J. Biol. Chem.* (1997) 272(38):23799-23804
- 30 32. Kamei, Y., Xu, L., Heinzl, T., Torchia, J., Kurokawa, R., Gloss, B., Lin, S. C., Heyman, R. A., Rose, D. W., Glass, C. K., and Rosenfeld, M. G. (1996). *Cell* 85, 403-14.
33. Kuiper, G. G., Carlsson, B., Grandien, K., Enmark, E., Haggblad, J., Nilsson, S., and Gustafsson, J. A. (1997). *Endocrinology* 138, 863-70.
34. Kuntz et al., *J. Mol. Biol.* (1982) 161:269-288
- 35 35. Kuntz et al., *Science*, (1992) 257:1078-1082
36. Kussie et al., *Science* (1996) 274:948-953

- 5 37. Landel, C., Kushner, P., and Greene, G. (1994). *Mol. Endocrinol.* 8, 1407-1419.
38. Landel, C., Potthoff, S., Nardulli, A., Kushner, J., and Greene, G. (1997). *J. Steroid Biochem. Molec. Biol.* 63, 59-73.
39. Lazennec, G., Ediger, T. R., Petz, L. N., Nardulli, A. M., and Katzenellenbogen, B. S. (1997). *Mol. Endocrinol.* 11, 1375-86.
- 10 40. Le Douarin, B., Nielsen, A. L., Garnier, J. M., Ichinose, H., Jeanmougin, F., Losson, R., and Chambon, P. (1996). *EMBO J* 15, 6701-15.
41. Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873
42. Lin et al., *Mol. Cell Biol.* (1997) 17(10):6131-6138
43. Masayama et al., *Mol. Endocrinol.* (1997) 11:1507-1517
- 15 44. Meng et al., *J. Comp. Chem.* (1992) 13:505-524
45. Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34
46. Muller, K., Amman, H. J., Doran, D. M., Gerber, P. R., Gubernator, K., and Schrepfer, G. (1988). *Bull. Soc. Chim. Belg.* 97, 655-667.
47. Murshudov, G. N., Vagin, A. A., and Dodson, E. J. (1997). *Acta Crystallogr. D* 53, 240-255.
- 20 48. Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210
49. Nishibata et al., *Tetrahedron* (1991) 47:8985;
50. Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073
51. Norris, J. D., Fan, D., Stallcup, M. R., and McDonnell, D. P. (1998). *J Biol Chem* 273, 6679-88.
52. O'Donnell et al., *Mol. Endocrinol.* (1991) 5:94-99
- 25 53. Onate et al., *Science* (1995) 270:1354-1357
54. Radhakrishnan et al., *Cell* (1997) 91:741-752
55. Renaud, J., Rochel, N., Ruff, M., Vivat, V., Chambon, P., Gronemeyer, H., and Moras, D. (1995). *Nature* 378, 681-689.
56. Saatcioglu et al., *Mol. Cell Biol.* (1997) 17:4687-4695
- 30 57. Sadovsky, et al., *Mol Cell Biol.* (1995) 15:1554
58. Seielstad, D., Carlson, K., Katzenellenbogen, J., Kushner, P., and Greene, G. (1995a). *Mol. Endocrinol.* 9, 647-658.
59. Seielstad, et al., *Biochemistry* (1995) 34:12605-12615
60. Shiau et al. *Gene* (1996) 179(2):205-10

- 5    61. Shibata et al., *Recent Prog. Horm. Res.* 52:141-164 (1997)
62. Spencer, T. E., Jenster, G., Burcin, M. M., Allis, C. D., Zhou, J., Mizzen, C. A., McKenna, N. J., Onate, S. A., Tsai, S. Y., Tsai, M. J., and O'Malley, B. W. (1997). *Nature* 389, 194-8.
63. Tagami et al., *Mol. Cell Biol.* (1997) 17(5):2642-2648
- 10    64. Tanenbaum, D. M., Wang, Y., Williams, S. P., and Sigler, P. B. (1998). *Proc. Natl. Acad. Sci. U S A* 95, 5998-6003.
65. Tora, L., Mullick, A., Metzger, D., Ponglikitmongkol, M., Park, I., and Chambon, P. (1989). *EMBO J* 8, 1981-6.
66. Torchia, J., Rose, D., Inostroza, J., Kamel, Y., Westin, S., Glass, C., and Rosenfeld, M. (1997). *Nature* 387, 677-684.
- 15    67. Uesugi et al., *Science* (1996) 277:1310-1313
68. Verlinde, *Structure*, (1994) 2:577-587)
69. Wagner, R., Apriletti, J., McGrath, M., West, B., Baxter, J., and Fletterick, R. (1995). *Nature* 378, 690-697.
70. Webb et al., *Mol Endocrinol* (1995) 9:443
- 20    71. White, R., Sjoberg, M., Kalkhoven, E., and Parker, M. G. (1997). *EMBO J* 16, 1427-35.
72. Whitfield et al., *Mol. Endocrinol.* (1995) 9:1166-79
73. Wurtz, J. M., Bourguet, W., Renaud, J. P., Vivat, V., Chambon, P., Moras, D., and Gronemeyer, H. (1996). *Nat. Struct. Biol.* 3, 87-94.
74. Zhu et al., *J. Biol. Chem.* (1997) 272(14):9048-9054

25

All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

5

## Appendix 1

Atomic Coordinates for Human TR- $\beta$  Complexed With T<sub>3</sub>, and a GRIP1 NR-box 2 Peptide

REMARK full length numbering  
 10 REMARK all residue names correct  
 REMARK peptide sequence  
 REMARK two molecules of TRB - CHAIN A and CHAIN B  
 REMARK two molecules of T<sub>3</sub> - CHAIN J and CHAIN K  
 REMARK two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y  
 15 REMARK chain X lies between A and B  
 REMARK chain Y interacts with B only  
 REMARK residues differing between A and B include:  
 REMARK A 217 Glu, A 252 Gln, A 263 Lys (missing side chains)  
 REMARK B 237 Ser, B239 His, B 394 Lys (missing side chains)  
 20 REMARK additionally Gly 261, Gly 262 are not visible in chain A  
 REMARK residues differing between X and Y include:  
 REMARK A 692 Arg  
 REMARK additionally, residues Lys 688, Lys 689; Ser 697, Ser 698  
 REMARK are not visible in chain Y

25	ATOM	1	N	LYS A 211	52.546	23.912	35.239	1.00	45.76	7
	ATOM	2	CA	LYS A 211	52.944	24.345	36.586	1.00	43.42	6
	ATOM	3	C	LYS A 211	52.035	23.665	37.836	1.00	35.68	6
	ATOM	4	O	LYS A 211	51.511	22.556	37.763	1.00	33.58	8
	ATOM	5	CB	LYS A 211	52.610	25.825	36.779	1.00	46.72	6
30	ATOM	6	N	PRO A 212	51.678	24.182	39.199	1.00	35.64	7
	ATOM	7	CD	PRO A 212	52.082	25.474	39.842	1.00	38.60	6
	ATOM	8	CA	PRO A 212	50.809	23.379	40.166	1.00	38.35	6
	ATOM	9	CB	PRO A 212	50.670	24.194	41.440	1.00	38.95	6
	ATOM	10	CG	PRO A 212	51.455	25.469	41.255	1.00	42.00	6
35	ATOM	11	C	PRO A 212	49.433	23.097	39.594	1.00	38.78	6
	ATOM	12	O	PRO A 212	48.920	23.949	38.802	1.00	34.64	8
	ATOM	13	N	GLU A 213	48.901	21.948	40.014	1.00	40.31	7
	ATOM	14	CA	GLU A 213	47.609	21.419	39.529	1.00	43.87	6
	ATOM	15	CB	GLU A 213	47.943	20.307	38.520	1.00	45.16	6
40	ATOM	16	CG	GLU A 213	49.125	20.708	37.601	1.00	47.60	6
	ATOM	17	CD	GLU A 213	49.284	19.828	36.353	1.00	50.68	6
	ATOM	18	OE1	GLU A 213	49.355	18.547	36.474	1.00	59.18	8
	ATOM	19	OE2	GLU A 213	49.356	20.368	35.180	1.00	49.06	8
	ATOM	20	C	GLU A 213	46.711	20.988	40.747	1.00	45.96	6
45	ATOM	21	O	GLU A 213	47.111	21.136	41.910	1.00	43.13	8
	ATOM	22	N	PRO A 214	45.463	20.460	40.515	1.00	46.52	7
	ATOM	23	CD	PRO A 214	44.985	20.184	39.148	1.00	46.44	6
	ATOM	24	CA	PRO A 214	44.447	20.124	41.596	1.00	47.52	6
	ATOM	25	CB	PRO A 214	43.249	19.629	40.816	1.00	45.40	6
50	ATOM	26	CG	PRO A 214	43.588	19.674	39.327	1.00	49.89	6
	ATOM	27	C	PRO A 214	44.787	19.082	42.625	1.00	45.70	6
	ATOM	28	O	PRO A 214	45.816	18.466	42.535	1.00	44.49	8
	ATOM	29	N	THR A 215	43.915	18.876	43.606	1.00	45.24	7
	ATOM	30	CA	THR A 215	44.161	17.890	44.686	1.00	49.36	6
55	ATOM	31	CB	THR A 215	44.163	18.586	46.093	1.00	44.86	6
	ATOM	32	OG1	THR A 215	42.878	18.447	46.728	1.00	52.26	8
	ATOM	33	CG2	THR A 215	44.514	20.031	45.974	1.00	39.43	6
	ATOM	34	C	THR A 215	42.934	16.995	44.667	1.00	52.51	6

5	ATOM	35	O	THR A 215	41.816	17.501	44.691	1.00	53.48	8
	ATOM	36	N	ASP A 216	43.118	15.683	44.607	1.00	58.81	7
	ATOM	37	CA	ASP A 216	41.973	14.740	44.615	1.00	61.51	6
	ATOM	38	CB	ASP A 216	42.386	13.451	45.343	1.00	70.57	6
	ATOM	39	CG	ASP A 216	42.399	12.283	44.475	1.00	78.07	6
10	ATOM	40	OD1	ASP A 216	41.532	12.161	43.586	1.00	82.31	8
	ATOM	41	OD2	ASP A 216	43.293	11.436	44.684	1.00	86.55	8
	ATOM	42	C	ASP A 216	40.640	15.311	45.268	1.00	58.42	6
	ATOM	43	O	ASP A 216	39.598	14.840	44.924	1.00	56.85	8
	ATOM	44	N	GLU A 217	40.673	16.270	46.217	1.00	54.92	7
15	ATOM	45	CA	GLU A 217	39.502	16.937	46.856	1.00	53.37	6
	ATOM	46	CB	GLU A 217	39.943	17.459	48.216	1.00	51.02	6
	ATOM	47	C	GLU A 217	39.113	18.144	45.956	1.00	53.55	6
	ATOM	48	O	GLU A 217	37.905	18.394	45.695	1.00	54.33	8
	ATOM	49	N	GLU A 218	40.162	18.895	45.511	1.00	49.20	7
20	ATOM	50	CA	GLU A 218	39.933	20.073	44.661	1.00	45.94	6
	ATOM	51	CB	GLU A 218	41.232	20.855	44.304	1.00	43.43	6
	ATOM	52	CG	GLU A 218	41.907	21.579	45.479	1.00	40.86	6
	ATOM	53	CD	GLU A 218	43.061	22.446	45.074	1.00	39.88	6
	ATOM	54	OE1	GLU A 218	43.895	22.019	44.232	1.00	37.61	8
25	ATOM	55	OE2	GLU A 218	43.183	23.583	45.599	1.00	34.01	8
	ATOM	56	C	GLU A 218	39.249	19.647	43.390	1.00	44.71	6
	ATOM	57	O	GLU A 218	38.302	20.291	42.964	1.00	45.31	8
	ATOM	58	N	TRP A 219	39.720	18.553	42.797	1.00	44.02	7
	ATOM	59	CA	TRP A 219	39.109	18.061	41.574	1.00	46.97	6
30	ATOM	60	CB	TRP A 219	39.799	16.793	41.074	1.00	48.42	6
	ATOM	61	CG	TRP A 219	40.879	17.029	40.141	1.00	54.61	6
	ATOM	62	CD2	TRP A 219	40.755	17.256	38.733	1.00	55.24	6
	ATOM	63	CE2	TRP A 219	42.067	17.523	38.245	1.00	53.67	6
	ATOM	64	CE3	TRP A 219	39.691	17.234	37.828	1.00	54.55	6
35	ATOM	65	CD1	TRP A 219	42.159	17.159	40.447	1.00	55.75	6
	ATOM	66	NE1	TRP A 219	42.895	17.485	39.339	1.00	54.43	7
	ATOM	67	CZ2	TRP A 219	42.330	17.851	36.895	1.00	52.54	6
	ATOM	68	CZ3	TRP A 219	39.943	17.535	36.509	1.00	55.17	6
	ATOM	69	CH2	TRP A 219	41.239	17.820	36.029	1.00	55.59	6
40	ATOM	70	C	TRP A 219	37.646	17.743	41.812	1.00	47.32	6
	ATOM	71	O	TRP A 219	36.788	18.028	40.978	1.00	43.56	8
	ATOM	72	N	GLU A 220	37.376	17.142	42.965	1.00	49.91	7
	ATOM	73	CA	GLU A 220	36.021	16.769	43.316	1.00	53.57	6
	ATOM	74	CB	GLU A 220	36.052	16.055	44.649	1.00	58.18	6
45	ATOM	75	CG	GLU A 220	35.149	14.930	44.672	1.00	73.13	6
	ATOM	76	CD	GLU A 220	35.735	13.935	45.442	1.00	80.06	6
	ATOM	77	OE1	GLU A 220	36.886	13.575	45.173	1.00	82.12	8
	ATOM	78	OE2	GLU A 220	35.078	13.478	46.378	1.00	82.78	8
	ATOM	79	C	GLU A 220	35.161	18.026	43.381	1.00	50.51	6
50	ATOM	80	O	GLU A 220	33.991	18.010	42.995	1.00	49.94	8
	ATOM	81	N	LEU A 221	35.761	19.120	43.865	1.00	43.71	7
	ATOM	82	CA	LEU A 221	35.047	20.398	43.951	1.00	42.81	6
	ATOM	83	CB	LEU A 221	35.935	21.510	44.510	1.00	39.21	6
	ATOM	84	CG	LEU A 221	35.375	22.908	44.353	1.00	36.34	6
55	ATOM	85	CD1	LEU A 221	33.941	22.929	44.836	1.00	36.93	6
	ATOM	86	CD2	LEU A 221	36.226	23.910	45.122	1.00	24.18	6
	ATOM	87	C	LEU A 221	34.563	20.815	42.575	1.00	43.46	6
	ATOM	88	O	LEU A 221	33.392	21.104	42.395	1.00	45.25	8

5	ATOM	89	N	ILE	A	222	35.498	20.871	41.628	1.00	39.09	7
	ATOM	90	CA	ILE	A	222	35.192	21.226	40.254	1.00	35.47	6
	ATOM	91	CB	ILE	A	222	36.379	20.997	39.343	1.00	33.74	6
	ATOM	92	CG2	ILE	A	222	35.970	21.182	37.893	1.00	28.86	6
	ATOM	93	CG1	ILE	A	222	37.532	21.922	39.707	1.00	33.33	6
10	ATOM	94	CD1	ILE	A	222	38.804	21.586	39.004	1.00	34.85	6
	ATOM	95	C	ILE	A	222	34.067	20.365	39.735	1.00	34.26	6
	ATOM	96	O	ILE	A	222	33.033	20.873	39.319	1.00	31.90	8
	ATOM	97	N	LYS	A	223	34.301	19.058	39.750	1.00	39.49	7
	ATOM	98	CA	LYS	A	223	33.316	18.100	39.276	1.00	44.43	6
15	ATOM	99	CB	LYS	A	223	33.603	16.713	39.852	1.00	50.81	6
	ATOM	100	CG	LYS	A	223	32.741	15.631	39.227	1.00	62.51	6
	ATOM	101	CD	LYS	A	223	32.859	14.291	39.943	1.00	72.22	6
	ATOM	102	CE	LYS	A	223	31.798	13.318	39.430	1.00	74.55	6
	ATOM	103	NZ	LYS	A	223	31.900	11.985	40.106	1.00	75.78	7
20	ATOM	104	C	LYS	A	223	31.913	18.565	39.681	1.00	42.81	6
	ATOM	105	O	LYS	A	223	30.936	18.323	38.984	1.00	40.36	8
	ATOM	106	N	THR	A	224	31.849	19.236	40.833	1.00	39.89	7
	ATOM	107	CA	THR	A	224	30.602	19.792	41.378	1.00	39.93	6
	ATOM	108	CB	THR	A	224	30.805	20.206	42.851	1.00	40.57	6
25	ATOM	109	OG1	THR	A	224	31.330	19.113	43.616	1.00	39.27	8
	ATOM	110	CG2	THR	A	224	29.500	20.684	43.461	1.00	38.11	6
	ATOM	111	C	THR	A	224	30.167	21.011	40.533	1.00	39.96	6
	ATOM	112	O	THR	A	224	29.313	20.899	39.655	1.00	36.67	8
	ATOM	113	N	VAL	A	225	30.777	22.160	40.832	1.00	38.02	7
30	ATOM	114	CA	VAL	A	225	30.532	23.426	40.137	1.00	38.12	6
	ATOM	115	CB	VAL	A	225	31.797	24.292	40.122	1.00	38.19	6
	ATOM	116	CG1	VAL	A	225	31.512	25.636	39.491	1.00	36.77	6
	ATOM	117	CG2	VAL	A	225	32.343	24.464	41.505	1.00	41.76	6
	ATOM	118	C	VAL	A	225	30.070	23.195	38.706	1.00	37.52	6
35	ATOM	119	O	VAL	A	225	29.119	23.803	38.239	1.00	36.77	8
	ATOM	120	N	THR	A	226	30.783	22.316	38.018	1.00	34.02	7
	ATOM	121	CA	THR	A	226	30.489	21.971	36.636	1.00	34.67	6
	ATOM	122	CB	THR	A	226	31.565	20.999	36.083	1.00	30.56	6
	ATOM	123	OG1	THR	A	226	32.805	21.696	35.889	1.00	32.20	8
40	ATOM	124	CG2	THR	A	226	31.108	20.346	34.783	1.00	20.99	6
	ATOM	125	C	THR	A	226	29.100	21.361	36.510	1.00	36.41	6
	ATOM	126	O	THR	A	226	28.255	21.877	35.785	1.00	39.64	8
	ATOM	127	N	ALA	A	227	28.880	20.260	37.222	1.00	39.20	7
	ATOM	128	CA	ALA	A	227	27.602	19.562	37.204	1.00	36.93	6
45	ATOM	129	CB	ALA	A	227	27.526	18.600	38.381	1.00	38.06	6
	ATOM	130	C	ALA	A	227	26.507	20.604	37.318	1.00	37.69	6
	ATOM	131	O	ALA	A	227	25.444	20.489	36.718	1.00	40.94	8
	ATOM	132	N	ALA	A	228	26.811	21.630	38.107	1.00	32.86	7
	ATOM	133	CA	ALA	A	228	25.903	22.734	38.356	1.00	32.48	6
50	ATOM	134	CB	ALA	A	228	26.448	23.587	39.486	1.00	28.25	6
	ATOM	135	C	ALA	A	228	25.732	23.570	37.101	1.00	36.12	6
	ATOM	136	O	ALA	A	228	24.673	23.560	36.473	1.00	37.86	8
	ATOM	137	N	HIS	A	229	26.782	24.306	36.752	1.00	33.58	7
	ATOM	138	CA	HIS	A	229	26.762	25.158	35.585	1.00	32.97	6
55	ATOM	139	CB	HIS	A	229	28.155	25.691	35.266	1.00	33.69	6
	ATOM	140	CG	HIS	A	229	28.250	26.333	33.929	1.00	28.39	6
	ATOM	141	CD2	HIS	A	229	29.025	26.081	32.838	1.00	28.83	6
	ATOM	142	ND1	HIS	A	229	27.386	27.368	33.542	1.00	30.47	7

5	ATOM	143	CE1	HIS	A	229	27.654	27.692	32.280	1.00	26.95	6
	ATOM	144	NE2	HIS	A	229	28.635	26.934	31.840	1.00	31.27	7
	ATOM	145	C	HIS	A	229	26.225	24.541	34.312	1.00	38.40	6
	ATOM	146	O	HIS	A	229	25.591	25.227	33.528	1.00	41.49	8
	ATOM	147	N	VAL	A	230	26.519	23.256	34.113	1.00	38.55	7
10	ATOM	148	CA	VAL	A	230	26.088	22.554	32.916	1.00	40.40	6
	ATOM	149	CB	VAL	A	230	26.890	21.256	32.701	1.00	44.68	6
	ATOM	150	CG1	VAL	A	230	26.557	20.656	31.345	1.00	39.39	6
	ATOM	151	CG2	VAL	A	230	28.381	21.509	32.817	1.00	42.18	6
	ATOM	152	C	VAL	A	230	24.603	22.239	32.900	1.00	44.28	6
15	ATOM	153	O	VAL	A	230	23.959	22.316	31.847	1.00	45.94	8
	ATOM	154	N	ALA	A	231	24.072	21.862	34.059	1.00	45.59	7
	ATOM	155	CA	ALA	A	231	22.669	21.500	34.175	1.00	47.84	6
	ATOM	156	CB	ALA	A	231	22.482	20.582	35.374	1.00	45.08	6
	ATOM	157	C	ALA	A	231	21.792	22.734	34.314	1.00	48.04	6
20	ATOM	158	O	ALA	A	231	20.565	22.647	34.324	1.00	49.95	8
	ATOM	159	N	THR	A	232	22.436	23.894	34.384	1.00	47.26	7
	ATOM	160	CA	THR	A	232	21.722	25.161	34.528	1.00	43.64	6
	ATOM	161	CB	THR	A	232	22.112	25.832	35.850	1.00	41.93	6
	ATOM	162	OG1	THR	A	232	23.467	26.283	35.791	1.00	39.10	8
25	ATOM	163	CG2	THR	A	232	21.990	24.846	37.008	1.00	29.80	6
	ATOM	164	C	THR	A	232	22.055	26.114	33.387	1.00	43.97	6
	ATOM	165	O	THR	A	232	21.679	27.279	33.436	1.00	40.55	8
	ATOM	166	N	ASN	A	233	22.783	25.625	32.381	1.00	48.62	7
	ATOM	167	CA	ASN	A	233	23.134	26.468	31.231	1.00	58.62	6
30	ATOM	168	CB	ASN	A	233	24.626	26.283	30.880	1.00	62.44	6
	ATOM	169	CG	ASN	A	233	25.141	27.355	29.927	1.00	68.35	6
	ATOM	170	OD1	ASN	A	233	24.822	28.544	30.096	1.00	65.50	8
	ATOM	171	ND2	ASN	A	233	25.951	26.951	28.959	1.00	74.29	7
	ATOM	172	C	ASN	A	233	22.241	26.035	30.073	1.00	65.06	6
35	ATOM	173	O	ASN	A	233	22.312	24.900	29.604	1.00	69.47	8
	ATOM	174	N	ALA	A	234	21.381	26.954	29.646	1.00	68.80	7
	ATOM	175	CA	ALA	A	234	20.423	26.708	28.564	1.00	70.98	6
	ATOM	176	CB	ALA	A	234	19.748	28.015	28.186	1.00	71.43	6
	ATOM	177	C	ALA	A	234	20.988	26.062	27.308	1.00	73.83	6
40	ATOM	178	O	ALA	A	234	22.041	26.419	26.822	1.00	74.33	8
	ATOM	179	N	GLN	A	235	20.227	25.096	26.819	1.00	75.07	7
	ATOM	180	CA	GLN	A	235	20.562	24.363	25.629	1.00	76.32	6
	ATOM	181	CB	GLN	A	235	20.328	25.239	24.391	1.00	76.98	6
	ATOM	182	CG	GLN	A	235	18.887	25.292	23.908	1.00	77.07	6
45	ATOM	183	CD	GLN	A	235	17.896	25.420	25.019	1.00	80.85	6
	ATOM	184	OE1	GLN	A	235	17.668	24.448	25.768	1.00	82.01	8
	ATOM	185	NE2	GLN	A	235	17.313	26.596	25.149	1.00	78.80	7
	ATOM	186	C	GLN	A	235	21.960	23.840	25.573	1.00	77.15	6
	ATOM	187	O	GLN	A	235	22.386	23.458	24.508	1.00	76.06	8
50	ATOM	188	N	GLY	A	236	22.676	23.766	26.687	1.00	77.46	7
	ATOM	189	CA	GLY	A	236	24.053	23.245	26.627	1.00	78.37	6
	ATOM	190	C	GLY	A	236	24.923	23.491	25.390	1.00	79.43	6
	ATOM	191	O	GLY	A	236	24.917	24.565	24.844	1.00	79.47	8
	ATOM	192	N	SER	A	237	25.739	22.526	24.991	1.00	77.98	7
55	ATOM	193	CA	SER	A	237	26.566	22.760	23.801	1.00	76.49	6
	ATOM	194	CB	SER	A	237	27.981	22.206	24.015	1.00	76.46	6
	ATOM	195	OG	SER	A	237	28.821	23.145	24.689	1.00	40.00	8
	ATOM	196	C	SER	A	237	25.938	22.127	22.542	1.00	75.35	6

5	ATOM	197	O	SER A 237	26.605	21.418	21.797	1.00	75.47	8
	ATOM	198	N	HIS A 238	24.648	22.410	22.353	1.00	75.56	7
	ATOM	199	CA	HIS A 238	23.842	21.981	21.236	1.00	75.46	6
	ATOM	200	CB	HIS A 238	22.990	20.732	21.661	1.00	75.85	6
	ATOM	201	CG	HIS A 238	22.408	19.933	20.542	1.00	40.00	6
10	ATOM	202	CD2	HIS A 238	22.790	18.757	19.957	1.00	40.00	6
	ATOM	203	ND1	HIS A 238	21.223	20.303	19.875	1.00	40.00	7
	ATOM	204	CE1	HIS A 238	20.951	19.365	18.953	1.00	40.00	6
	ATOM	205	NE2	HIS A 238	21.874	18.444	18.994	1.00	40.00	7
	ATOM	206	C	HIS A 238	22.971	23.284	20.964	1.00	74.10	6
15	ATOM	207	O	HIS A 238	21.863	23.137	20.441	1.00	75.34	8
	ATOM	208	N	TRP A 239	23.487	24.510	21.368	1.00	73.39	7
	ATOM	209	CA	TRP A 239	22.872	25.894	21.195	1.00	74.02	6
	ATOM	210	CB	TRP A 239	23.563	27.026	22.005	1.00	81.77	6
	ATOM	211	CG	TRP A 239	25.022	27.366	21.688	1.00	89.67	6
20	ATOM	212	CD2	TRP A 239	25.532	28.662	21.240	1.00	93.19	6
	ATOM	213	CE2	TRP A 239	26.961	28.522	21.136	1.00	95.46	6
	ATOM	214	CE3	TRP A 239	24.936	29.911	20.969	1.00	95.35	6
	ATOM	215	CD1	TRP A 239	26.102	26.548	21.781	1.00	94.16	6
	ATOM	216	NE1	TRP A 239	27.268	27.241	21.475	1.00	97.48	7
25	ATOM	217	CZ2	TRP A 239	27.798	29.598	20.764	1.00	96.23	6
	ATOM	218	CZ3	TRP A 239	25.763	30.967	20.569	1.00	96.75	6
	ATOM	219	CH2	TRP A 239	27.171	30.825	20.482	1.00	97.32	6
	ATOM	220	C	TRP A 239	22.799	26.407	19.774	1.00	70.77	6
	ATOM	221	O	TRP A 239	21.706	26.562	19.263	1.00	71.70	8
30	ATOM	222	N	LYS A 240	23.946	26.701	19.157	1.00	67.10	7
	ATOM	223	CA	LYS A 240	23.978	27.180	17.783	1.00	65.63	6
	ATOM	224	CB	LYS A 240	25.314	26.780	17.153	1.00	66.65	6
	ATOM	225	CG	LYS A 240	26.529	27.342	17.872	1.00	69.83	6
	ATOM	226	CD	LYS A 240	27.805	27.037	17.108	1.00	71.49	6
35	ATOM	227	CE	LYS A 240	28.980	27.720	17.776	1.00	71.31	6
	ATOM	228	NZ	LYS A 240	30.238	27.438	17.034	1.00	72.23	7
	ATOM	229	C	LYS A 240	22.808	26.699	16.895	1.00	66.19	6
	ATOM	230	O	LYS A 240	22.550	27.298	15.851	1.00	65.20	8
	ATOM	231	N	ASN A 241	22.113	25.640	17.325	1.00	66.69	7
40	ATOM	232	CA	ASN A 241	20.976	25.078	16.599	1.00	67.53	6
	ATOM	233	CB	ASN A 241	21.122	23.562	16.550	1.00	67.98	6
	ATOM	234	CG	ASN A 241	22.304	23.121	15.693	1.00	70.19	6
	ATOM	235	OD1	ASN A 241	22.404	23.506	14.503	1.00	71.37	8
	ATOM	236	ND2	ASN A 241	23.176	22.310	16.271	1.00	71.48	7
45	ATOM	237	C	ASN A 241	19.570	25.421	17.152	1.00	66.62	6
	ATOM	238	O	ASN A 241	18.581	24.822	16.731	1.00	64.76	8
	ATOM	239	N	LYS A 242	19.475	26.380	18.069	1.00	66.86	7
	ATOM	240	CA	LYS A 242	18.191	26.786	18.642	1.00	67.46	6
	ATOM	241	CB	LYS A 242	18.164	26.396	20.119	1.00	67.93	6
50	ATOM	242	CG	LYS A 242	18.250	24.896	20.337	1.00	71.52	6
	ATOM	243	CD	LYS A 242	17.004	24.149	19.821	1.00	74.32	6
	ATOM	244	CE	LYS A 242	15.755	24.491	20.643	1.00	74.41	6
	ATOM	245	NZ	LYS A 242	15.927	24.161	22.109	1.00	74.44	7
	ATOM	246	C	LYS A 242	18.143	28.291	18.483	1.00	66.28	6
55	ATOM	247	O	LYS A 242	17.102	28.923	18.592	1.00	67.61	8
	ATOM	248	N	ARG A 243	19.334	28.813	18.204	1.00	64.19	7
	ATOM	249	CA	ARG A 243	19.617	30.219	17.975	1.00	62.43	6
	ATOM	250	CB	ARG A 243	21.070	30.274	17.463	1.00	60.12	6



5	ATOM	251	CG	ARG	A	243	21.665	31.636	17.305	1.00	40.00	6
	ATOM	252	CD	ARG	A	243	23.213	31.599	17.267	1.00	40.00	6
	ATOM	253	NE	ARG	A	243	23.826	31.217	15.996	1.00	40.00	7
	ATOM	254	CZ	ARG	A	243	25.113	31.439	15.714	1.00	40.00	6
	ATOM	255	NH1	ARG	A	243	25.905	32.041	16.616	1.00	40.00	7
10	ATOM	256	NH2	ARG	A	243	25.592	31.097	14.520	1.00	40.00	7
	ATOM	257	C	ARG	A	243	18.639	30.789	16.950	1.00	62.97	6
	ATOM	258	O	ARG	A	243	18.662	30.390	15.784	1.00	63.96	8
	ATOM	259	N	LYS	A	244	17.771	31.692	17.393	1.00	62.41	7
	ATOM	260	CA	LYS	A	244	16.790	32.309	16.498	1.00	61.57	6
15	ATOM	261	CB	LYS	A	244	15.368	31.974	16.962	1.00	63.68	6
	ATOM	262	CG	LYS	A	244	15.102	30.471	17.104	1.00	71.29	6
	ATOM	263	CD	LYS	A	244	13.641	30.167	17.468	1.00	73.83	6
	ATOM	264	CE	LYS	A	244	13.182	30.908	18.737	1.00	74.71	6
	ATOM	265	NZ	LYS	A	244	13.951	30.536	19.970	1.00	73.32	7
20	ATOM	266	C	LYS	A	244	17.009	33.806	16.501	1.00	59.30	6
	ATOM	267	O	LYS	A	244	16.562	34.514	17.399	1.00	56.34	8
	ATOM	268	N	PHE	A	245	17.705	34.264	15.468	1.00	57.06	7
	ATOM	269	CA	PHE	A	245	18.045	35.692	15.333	1.00	59.01	6
	ATOM	270	CB	PHE	A	245	18.825	35.947	14.049	1.00	59.62	6
25	ATOM	271	CG	PHE	A	245	19.908	34.979	13.834	1.00	66.60	6
	ATOM	272	CD1	PHE	A	245	19.618	33.714	13.399	1.00	67.17	6
	ATOM	273	CD2	PHE	A	245	21.198	35.309	14.139	1.00	69.25	6
	ATOM	274	CE1	PHE	A	245	20.614	32.794	13.255	1.00	69.92	6
	ATOM	275	CE2	PHE	A	245	22.189	34.385	13.994	1.00	70.50	6
30	ATOM	276	CZ	PHE	A	245	21.897	33.126	13.552	1.00	70.89	6
	ATOM	277	C	PHE	A	245	16.856	36.620	15.340	1.00	60.68	6
	ATOM	278	O	PHE	A	245	15.946	36.516	14.528	1.00	62.37	8
	ATOM	279	N	LEU	A	246	16.919	37.558	16.272	1.00	60.10	7
	ATOM	280	CA	LEU	A	246	15.884	38.554	16.437	1.00	59.44	6
35	ATOM	281	CB	LEU	A	246	16.227	39.510	17.585	1.00	57.43	6
	ATOM	282	CG	LEU	A	246	15.100	40.384	18.086	1.00	54.41	6
	ATOM	283	CD1	LEU	A	246	14.010	39.474	18.640	1.00	52.43	6
	ATOM	284	CD2	LEU	A	246	15.575	41.325	19.151	1.00	51.69	6
	ATOM	285	C	LEU	A	246	15.717	39.330	15.135	1.00	62.05	6
40	ATOM	286	O	LEU	A	246	16.706	39.609	14.430	1.00	59.85	8
	ATOM	287	N	PRO	A	247	14.473	39.668	14.784	1.00	63.33	7
	ATOM	288	CD	PRO	A	247	13.263	39.314	15.534	1.00	64.44	6
	ATOM	289	CA	PRO	A	247	14.198	40.421	13.558	1.00	63.56	6
	ATOM	290	CB	PRO	A	247	12.687	40.671	13.600	1.00	64.42	6
45	ATOM	291	CG	PRO	A	247	12.161	39.922	14.729	1.00	64.90	6
	ATOM	292	C	PRO	A	247	14.996	41.733	13.496	1.00	61.94	6
	ATOM	293	O	PRO	A	247	15.159	42.455	14.486	1.00	61.60	8
	ATOM	294	N	GLU	A	248	15.506	42.006	12.299	1.00	61.33	7
	ATOM	295	CA	GLU	A	248	16.280	43.197	11.976	1.00	63.50	6
50	ATOM	296	CB	GLU	A	248	16.481	43.273	10.437	1.00	66.94	6
	ATOM	297	CG	GLU	A	248	17.012	44.671	9.966	1.00	68.70	6
	ATOM	298	CD	GLU	A	248	16.981	44.939	8.471	1.00	40.00	6
	ATOM	299	OE1	GLU	A	248	16.432	44.144	7.644	1.00	40.00	8
	ATOM	300	OE2	GLU	A	248	17.509	46.015	8.086	1.00	40.00	8
55	ATOM	301	C	GLU	A	248	15.624	44.489	12.458	1.00	64.19	6
	ATOM	302	O	GLU	A	248	16.298	45.395	12.918	1.00	65.56	8
	ATOM	303	N	ASP	A	249	14.300	44.545	12.323	1.00	64.36	7
	ATOM	304	CA	ASP	A	249	13.493	45.703	12.673	1.00	63.33	6

5	ATOM	305	CB	ASP	A	249	12.088	45.531	12.116	1.00	62.97	6
	ATOM	306	CG	ASP	A	249	11.277	44.527	12.870	1.00	64.63	6
	ATOM	307	OD1	ASP	A	249	11.687	43.352	12.963	1.00	64.84	8
	ATOM	308	OD2	ASP	A	249	10.183	44.880	13.395	1.00	66.52	8
	ATOM	309	C	ASP	A	249	13.371	46.062	14.130	1.00	64.31	6
10	ATOM	310	O	ASP	A	249	13.310	47.250	14.468	1.00	64.73	8
	ATOM	311	N	ILE	A	250	13.274	45.049	14.997	1.00	63.09	7
	ATOM	312	CA	ILE	A	250	13.133	45.318	16.418	1.00	64.39	6
	ATOM	313	CB	ILE	A	250	13.035	44.034	17.214	1.00	65.79	6
	ATOM	314	CG2	ILE	A	250	12.001	44.104	18.336	1.00	64.78	6
15	ATOM	315	CG1	ILE	A	250	12.611	42.860	16.341	1.00	65.28	6
	ATOM	316	CD1	ILE	A	250	11.753	41.852	17.088	1.00	65.08	6
	ATOM	317	C	ILE	A	250	14.404	46.104	17.276	1.00	65.21	6
	ATOM	318	O	ILE	A	250	15.155	45.506	18.047	1.00	64.05	8
	ATOM	319	N	GLY	A	251	14.670	47.529	17.299	1.00	65.48	7
20	ATOM	320	CA	GLY	A	251	15.871	48.326	18.042	1.00	67.32	6
	ATOM	321	C	GLY	A	251	16.595	49.110	16.895	1.00	68.52	6
	ATOM	322	O	GLY	A	251	17.528	48.616	16.266	1.00	65.49	8
	ATOM	323	N	GLN	A	252	16.162	50.356	16.557	1.00	72.26	7
	ATOM	324	CA	GLN	A	252	16.541	50.930	15.207	1.00	74.10	6
25	ATOM	325	CB	GLN	A	252	15.316	50.844	14.295	1.00	75.82	6
	ATOM	326	C	GLN	A	252	16.995	52.403	15.084	1.00	77.17	6
	ATOM	327	O	GLN	A	252	17.572	52.955	15.986	1.00	76.50	8
	ATOM	328	N	ALA	A	253	16.374	53.372	13.908	1.00	80.78	7
	ATOM	329	CA	ALA	A	253	16.687	54.725	13.567	1.00	83.70	6
30	ATOM	330	CB	ALA	A	253	16.381	54.956	12.093	1.00	83.23	6
	ATOM	331	C	ALA	A	253	16.159	55.960	14.345	1.00	85.59	6
	ATOM	332	O	ALA	A	253	15.317	56.721	13.798	1.00	85.69	8
	ATOM	333	N	PRO	A	254	16.384	56.155	16.264	1.00	35.05	7
	ATOM	334	CD	PRO	A	254	17.102	55.053	16.908	1.00	33.97	6
35	ATOM	335	CA	PRO	A	254	16.002	57.231	17.219	1.00	35.89	6
	ATOM	336	CB	PRO	A	254	16.534	56.756	18.563	1.00	33.94	6
	ATOM	337	CG	PRO	A	254	17.146	55.441	18.349	1.00	33.31	6
	ATOM	338	C	PRO	A	254	16.717	58.498	16.731	1.00	37.75	6
	ATOM	339	O	PRO	A	254	17.838	58.804	17.100	1.00	38.78	8
40	TER											
	ATOM	1	N	LYS	A	263	18.045	57.462	23.875	1.00	61.71	7
	ATOM	2	CA	LYS	A	263	16.824	56.712	24.215	1.00	64.36	6
	ATOM	3	CB	LYS	A	263	15.758	57.004	23.141	1.00	63.50	6
	ATOM	4	C	LYS	A	263	16.841	55.180	24.429	1.00	63.41	6
45	ATOM	5	O	LYS	A	263	17.877	54.542	24.409	1.00	61.93	8
	ATOM	6	N	VAL	A	264	15.615	54.664	24.654	1.00	61.15	7
	ATOM	7	CA	VAL	A	264	15.292	53.229	24.856	1.00	59.46	6
	ATOM	8	CB	VAL	A	264	14.251	52.974	25.978	1.00	59.03	6
	ATOM	9	CG1	VAL	A	264	14.229	51.494	26.368	1.00	53.79	6
50	ATOM	10	CG2	VAL	A	264	14.449	53.818	27.142	1.00	55.32	6
	ATOM	11	C	VAL	A	264	14.590	52.820	23.554	1.00	60.96	6
	ATOM	12	O	VAL	A	264	14.734	53.468	22.508	1.00	62.13	8
	ATOM	13	N	ASP	A	265	13.802	51.755	23.634	1.00	62.59	7
	ATOM	14	CA	ASP	A	265	12.995	51.263	22.526	1.00	64.95	6
55	ATOM	15	CB	ASP	A	265	13.825	51.077	21.271	1.00	64.32	6
	ATOM	16	CG	ASP	A	265	13.282	50.048	20.485	1.00	67.70	6
	ATOM	17	OD1	ASP	A	265	12.795	50.011	19.446	1.00	72.59	8
	ATOM	18	OD2	ASP	A	265	13.354	48.867	20.294	1.00	68.84	8

5	ATOM	19	C	ASP A 265	12.326	49.943	22.952	1.00	65.64	6
	ATOM	20	O	ASP A 265	12.771	48.850	22.655	1.00	68.81	8
	ATOM	21	N	LEU A 266	11.256	50.152	23.702	1.00	65.12	7
	ATOM	22	CA	LEU A 266	10.368	49.169	24.288	1.00	63.40	6
	ATOM	23	CB	LEU A 266	9.115	49.938	24.708	1.00	67.34	6
10	ATOM	24	CG	LEU A 266	9.399	51.124	25.618	1.00	69.35	6
	ATOM	25	CD1	LEU A 266	8.304	52.148	25.533	1.00	68.24	6
	ATOM	26	CD2	LEU A 266	9.581	50.631	27.021	1.00	70.47	6
	ATOM	27	C	LEU A 266	9.940	47.888	23.559	1.00	59.67	6
	ATOM	28	O	LEU A 266	9.694	46.879	24.220	1.00	53.35	8
15	ATOM	29	N	GLU A 267	9.815	47.904	22.235	1.00	58.01	7
	ATOM	30	CA	GLU A 267	9.417	46.682	21.572	1.00	58.34	6
	ATOM	31	CB	GLU A 267	9.311	46.855	20.048	1.00	59.21	6
	ATOM	32	CG	GLU A 267	9.129	45.494	19.322	1.00	62.89	6
	ATOM	33	CD	GLU A 267	8.736	45.592	17.883	1.00	67.66	6
20	ATOM	34	OE1	GLU A 267	9.433	46.263	17.080	1.00	69.95	8
	ATOM	35	OE2	GLU A 267	7.710	44.974	17.503	1.00	69.40	8
	ATOM	36	C	GLU A 267	10.504	45.683	21.895	1.00	57.67	6
	ATOM	37	O	GLU A 267	10.255	44.485	21.988	1.00	58.34	8
	ATOM	38	N	ALA A 268	11.712	46.222	22.054	1.00	53.43	7
25	ATOM	39	CA	ALA A 268	12.903	45.454	22.374	1.00	49.00	6
	ATOM	40	CB	ALA A 268	14.137	46.241	21.983	1.00	45.72	6
	ATOM	41	C	ALA A 268	12.908	45.196	23.873	1.00	45.76	6
	ATOM	42	O	ALA A 268	12.887	44.042	24.307	1.00	41.50	8
	ATOM	43	N	PHE A 269	12.918	46.277	24.663	1.00	41.43	7
30	ATOM	44	CA	PHE A 269	12.920	46.158	26.118	1.00	43.96	6
	ATOM	45	CB	PHE A 269	12.395	47.426	26.777	1.00	40.10	6
	ATOM	46	CG	PHE A 269	12.332	47.345	28.271	1.00	40.44	6
	ATOM	47	CD1	PHE A 269	13.457	47.595	29.034	1.00	38.98	6
	ATOM	48	CD2	PHE A 269	11.165	46.946	28.903	1.00	37.15	6
35	ATOM	49	CE1	PHE A 269	13.409	47.469	30.436	1.00	32.12	6
	ATOM	50	CE2	PHE A 269	11.105	46.815	30.303	1.00	38.41	6
	ATOM	51	CZ	PHE A 269	12.228	47.070	31.071	1.00	40.55	6
	ATOM	52	C	PHE A 269	12.017	45.012	26.520	1.00	49.76	6
	ATOM	53	O	PHE A 269	12.277	44.324	27.484	1.00	52.15	8
40	ATOM	54	N	SER A 270	10.934	44.835	25.768	1.00	53.15	7
	ATOM	55	CA	SER A 270	9.988	43.768	26.043	1.00	52.29	6
	ATOM	56	CB	SER A 270	8.727	43.943	25.215	1.00	51.85	6
	ATOM	57	OG	SER A 270	7.785	42.918	25.497	1.00	53.42	8
	ATOM	58	C	SER A 270	10.637	42.464	25.685	1.00	49.38	6
45	ATOM	59	O	SER A 270	11.068	41.741	26.562	1.00	48.74	8
	ATOM	60	N	HIS A 271	10.683	42.173	24.383	1.00	50.15	7
	ATOM	61	CA	HIS A 271	11.276	40.932	23.877	1.00	51.67	6
	ATOM	62	CB	HIS A 271	11.797	41.118	22.455	1.00	58.52	6
	ATOM	63	CG	HIS A 271	10.775	40.885	21.399	1.00	68.97	6
50	ATOM	64	CD2	HIS A 271	10.633	39.891	20.485	1.00	70.88	6
	ATOM	65	ND1	HIS A 271	9.673	41.732	21.199	1.00	71.98	7
	ATOM	66	CE1	HIS A 271	8.936	41.242	20.209	1.00	73.91	6
	ATOM	67	NE2	HIS A 271	9.495	40.132	19.764	1.00	73.59	7
	ATOM	68	C	HIS A 271	12.402	40.416	24.745	1.00	48.33	6
55	ATOM	69	O	HIS A 271	12.707	39.225	24.728	1.00	48.39	8
	ATOM	70	N	PHE A 272	13.029	41.334	25.487	1.00	41.34	7
	ATOM	71	CA	PHE A 272	14.130	41.001	26.384	1.00	39.44	6
	ATOM	72	CB	PHE A 272	15.077	42.194	26.512	1.00	36.67	6

5	ATOM	73	CG	PHE	A	272	15.953	42.413	25.282	1.00	33.39	6
	ATOM	74	CD1	PHE	A	272	16.619	43.615	25.093	1.00	33.14	6
	ATOM	75	CD2	PHE	A	272	16.138	41.394	24.346	1.00	38.28	6
	ATOM	76	CE1	PHE	A	272	17.454	43.807	23.988	1.00	38.26	6
	ATOM	77	CE2	PHE	A	272	16.973	41.585	23.244	1.00	43.28	6
10	ATOM	78	CZ	PHE	A	272	17.634	42.786	23.068	1.00	39.74	6
	ATOM	79	C	PHE	A	272	13.650	40.528	27.764	1.00	40.75	6
	ATOM	80	O	PHE	A	272	14.081	39.476	28.227	1.00	35.51	8
	ATOM	81	N	THR	A	273	12.756	41.266	28.428	1.00	41.64	7
	ATOM	82	CA	THR	A	273	12.290	40.854	29.757	1.00	45.97	6
15	ATOM	83	CB	THR	A	273	11.651	42.025	30.506	1.00	51.52	6
	ATOM	84	OG1	THR	A	273	10.442	42.422	29.859	1.00	45.74	8
	ATOM	85	CG2	THR	A	273	12.601	43.211	30.565	1.00	49.73	6
	ATOM	86	C	THR	A	273	11.267	39.731	29.664	1.00	46.23	6
	ATOM	87	O	THR	A	273	10.854	39.183	30.680	1.00	41.21	8
20	ATOM	88	N	LYS	A	274	10.849	39.412	28.440	1.00	46.21	7
	ATOM	89	CA	LYS	A	274	9.871	38.362	28.211	1.00	54.53	6
	ATOM	90	CB	LYS	A	274	9.414	38.405	26.773	1.00	54.36	6
	ATOM	91	C	LYS	A	274	10.498	37.015	28.515	1.00	56.88	6
	ATOM	92	O	LYS	A	274	9.789	36.044	28.759	1.00	57.98	8
25	ATOM	93	N	ILE	A	275	11.836	36.973	28.491	1.00	56.48	7
	ATOM	94	CA	ILE	A	275	12.609	35.746	28.767	1.00	52.64	6
	ATOM	95	CB	ILE	A	275	13.444	35.346	27.543	1.00	49.15	6
	ATOM	96	CG2	ILE	A	275	12.568	34.829	26.429	1.00	47.42	6
	ATOM	97	CG1	ILE	A	275	14.238	36.532	27.026	1.00	45.31	6
30	ATOM	98	CD1	ILE	A	275	15.001	36.242	25.771	1.00	37.22	6
	ATOM	99	C	ILE	A	275	13.541	35.870	29.982	1.00	51.78	6
	ATOM	100	O	ILE	A	275	14.014	34.873	30.503	1.00	49.80	8
	ATOM	101	N	ILE	A	276	13.790	37.107	30.415	1.00	51.76	7
	ATOM	102	CA	ILE	A	276	14.681	37.389	31.537	1.00	52.58	6
35	ATOM	103	CB	ILE	A	276	14.691	38.877	31.844	1.00	55.04	6
	ATOM	104	CG2	ILE	A	276	13.311	39.340	32.261	1.00	53.28	6
	ATOM	105	CG1	ILE	A	276	15.675	39.206	32.976	1.00	57.31	6
	ATOM	106	CD1	ILE	A	276	17.096	38.942	32.655	1.00	60.32	6
	ATOM	107	C	ILE	A	276	14.323	36.644	32.828	1.00	50.70	6
40	ATOM	108	O	ILE	A	276	15.177	36.458	33.691	1.00	55.55	8
	ATOM	109	N	THR	A	277	13.072	36.209	32.963	1.00	47.33	7
	ATOM	110	CA	THR	A	277	12.631	35.523	34.158	1.00	42.59	6
	ATOM	111	CB	THR	A	277	11.098	35.456	34.217	1.00	44.97	6
	ATOM	112	OG1	THR	A	277	10.545	36.777	34.102	1.00	46.38	8
45	ATOM	113	CG2	THR	A	277	10.657	34.838	35.539	1.00	37.17	6
	ATOM	114	C	THR	A	277	13.211	34.118	34.304	1.00	39.84	6
	ATOM	115	O	THR	A	277	13.796	33.796	35.365	1.00	40.55	8
	ATOM	116	N	PRO	A	278	13.055	33.261	33.288	1.00	38.20	7
	ATOM	117	CD	PRO	A	278	12.370	33.534	32.023	1.00	36.34	6
50	ATOM	118	CA	PRO	A	278	13.595	31.894	33.363	1.00	36.63	6
	ATOM	119	CB	PRO	A	278	13.153	31.244	32.064	1.00	32.95	6
	ATOM	120	CG	PRO	A	278	12.573	32.291	31.239	1.00	35.75	6
	ATOM	121	C	PRO	A	278	15.101	31.932	33.476	1.00	38.60	6
	ATOM	122	O	PRO	A	278	15.746	30.981	33.898	1.00	37.67	8
55	ATOM	123	N	ALA	A	279	15.656	33.051	33.035	1.00	37.05	7
	ATOM	124	CA	ALA	A	279	17.087	33.277	33.041	1.00	33.18	6
	ATOM	125	CB	ALA	A	279	17.376	34.599	32.348	1.00	30.56	6
	ATOM	126	C	ALA	A	279	17.624	33.312	34.452	1.00	33.47	6

5	ATOM	127	O	ALA	A	279	18.523	32.555	34.789	1.00	33.74	8
	ATOM	128	N	ILE	A	280	17.060	34.215	35.260	1.00	29.96	7
	ATOM	129	CA	ILE	A	280	17.459	34.362	36.646	1.00	25.94	6
	ATOM	130	CB	ILE	A	280	16.686	35.484	37.315	1.00	26.95	6
	ATOM	131	CG2	ILE	A	280	17.109	35.632	38.733	1.00	15.40	6
10	ATOM	132	CG1	ILE	A	280	16.931	36.808	36.595	1.00	26.73	6
	ATOM	133	CD1	ILE	A	280	16.292	38.002	37.272	1.00	34.31	6
	ATOM	134	C	ILE	A	280	17.263	33.066	37.412	1.00	31.39	6
	ATOM	135	O	ILE	A	280	18.116	32.679	38.207	1.00	35.69	8
	ATOM	136	N	THR	A	281	16.145	32.386	37.165	1.00	30.90	7
15	ATOM	137	CA	THR	A	281	15.854	31.118	37.851	1.00	33.49	6
	ATOM	138	CB	THR	A	281	14.598	30.413	37.277	1.00	37.18	6
	ATOM	139	OG1	THR	A	281	14.795	30.099	35.898	1.00	46.48	8
	ATOM	140	CG2	THR	A	281	13.352	31.281	37.444	1.00	32.85	6
	ATOM	141	C	THR	A	281	17.045	30.176	37.713	1.00	29.94	6
20	ATOM	142	O	THR	A	281	17.478	29.546	38.684	1.00	25.55	8
	ATOM	143	N	ARG	A	282	17.561	30.076	36.489	1.00	32.70	7
	ATOM	144	CA	ARG	A	282	18.692	29.198	36.218	1.00	34.27	6
	ATOM	145	CB	ARG	A	282	19.136	29.374	34.780	1.00	33.78	6
	ATOM	146	CG	ARG	A	282	19.272	28.086	34.013	1.00	45.15	6
25	ATOM	147	CD	ARG	A	282	18.179	27.921	32.977	1.00	58.24	6
	ATOM	148	NE	ARG	A	282	18.041	29.077	32.117	1.00	68.41	7
	ATOM	149	CZ	ARG	A	282	19.018	29.529	31.352	1.00	72.31	6
	ATOM	150	NH1	ARG	A	282	20.190	28.886	31.327	1.00	77.89	7
	ATOM	151	NH2	ARG	A	282	18.802	30.593	30.595	1.00	69.25	7
30	ATOM	152	C	ARG	A	282	19.823	29.582	37.170	1.00	34.81	6
	ATOM	153	O	ARG	A	282	20.380	28.735	37.855	1.00	36.03	8
	ATOM	154	N	VAL	A	283	20.135	30.882	37.190	1.00	31.71	7
	ATOM	155	CA	VAL	A	283	21.171	31.434	38.057	1.00	30.16	6
	ATOM	156	CB	VAL	A	283	21.198	32.965	37.981	1.00	29.00	6
35	ATOM	157	CG1	VAL	A	283	22.208	33.533	38.952	1.00	28.64	6
	ATOM	158	CG2	VAL	A	283	21.525	33.415	36.578	1.00	28.28	6
	ATOM	159	C	VAL	A	283	20.942	30.992	39.498	1.00	32.50	6
	ATOM	160	O	VAL	A	283	21.879	30.717	40.229	1.00	33.48	8
	ATOM	161	N	VAL	A	284	19.671	30.941	39.892	1.00	30.96	7
40	ATOM	162	CA	VAL	A	284	19.289	30.527	41.239	1.00	29.14	6
	ATOM	163	CB	VAL	A	284	17.822	30.865	41.548	1.00	31.27	6
	ATOM	164	CG1	VAL	A	284	17.472	30.461	42.945	1.00	24.21	6
	ATOM	165	CG2	VAL	A	284	17.555	32.334	41.360	1.00	30.51	6
	ATOM	166	C	VAL	A	284	19.529	29.037	41.353	1.00	28.89	6
45	ATOM	167	O	VAL	A	284	20.073	28.568	42.345	1.00	27.29	8
	ATOM	168	N	ASP	A	285	19.121	28.296	40.327	1.00	28.76	7
	ATOM	169	CA	ASP	A	285	19.277	26.842	40.306	1.00	35.32	6
	ATOM	170	CB	ASP	A	285	18.586	26.234	39.072	1.00	33.29	6
	ATOM	171	CG	ASP	A	285	17.083	26.277	39.149	1.00	38.15	6
50	ATOM	172	OD1	ASP	A	285	16.484	25.743	40.110	1.00	34.70	8
	ATOM	173	OD2	ASP	A	285	16.431	26.828	38.231	1.00	34.43	8
	ATOM	174	C	ASP	A	285	20.751	26.449	40.305	1.00	36.70	6
	ATOM	175	O	ASP	A	285	21.106	25.389	40.808	1.00	37.96	8
	ATOM	176	N	PHE	A	286	21.604	27.300	39.737	1.00	35.96	7
55	ATOM	177	CA	PHE	A	286	23.029	27.022	39.704	1.00	37.10	6
	ATOM	178	CB	PHE	A	286	23.754	28.009	38.793	1.00	37.97	6
	ATOM	179	CG	PHE	A	286	25.252	28.027	38.987	1.00	36.50	6
	ATOM	180	CD1	PHE	A	286	25.963	26.849	38.974	1.00	36.75	6

5	ATOM	181	CD2	PHE A 286	25.931	29.218	39.199	1.00	33.83	6
	ATOM	182	CE1	PHE A 286	27.331	26.860	39.161	1.00	39.55	6
	ATOM	183	CE2	PHE A 286	27.307	29.233	39.387	1.00	38.08	6
	ATOM	184	CZ	PHE A 286	28.008	28.052	39.371	1.00	34.44	6
	ATOM	185	C	PHE A 286	23.631	27.105	41.083	1.00	36.83	6
10	ATOM	186	O	PHE A 286	24.317	26.192	41.504	1.00	35.61	8
	ATOM	187	N	ALA A 287	23.393	28.228	41.752	1.00	37.33	7
	ATOM	188	CA	ALA A 287	23.917	28.448	43.087	1.00	36.34	6
	ATOM	189	CB	ALA A 287	23.523	29.828	43.555	1.00	36.40	6
	ATOM	190	C	ALA A 287	23.346	27.393	44.027	1.00	38.76	6
15	ATOM	191	O	ALA A 287	23.994	26.973	44.981	1.00	41.98	8
	ATOM	192	N	LYS A 288	22.114	26.979	43.735	1.00	38.28	7
	ATOM	193	CA	LYS A 288	21.429	25.971	44.538	1.00	45.26	6
	ATOM	194	CB	LYS A 288	19.994	25.746	44.054	1.00	48.35	6
	ATOM	195	CG	LYS A 288	19.025	26.819	44.464	1.00	51.43	6
20	ATOM	196	CD	LYS A 288	17.628	26.246	44.682	1.00	60.23	6
	ATOM	197	CE	LYS A 288	17.135	25.478	43.485	1.00	62.81	6
	ATOM	198	NZ	LYS A 288	17.196	26.327	42.268	1.00	64.69	7
	ATOM	199	C	LYS A 288	22.120	24.632	44.536	1.00	43.31	6
	ATOM	200	O	LYS A 288	21.967	23.857	45.462	1.00	45.66	8
25	ATOM	201	N	LYS A 289	22.865	24.366	43.467	1.00	41.70	7
	ATOM	202	CA	LYS A 289	23.571	23.120	43.351	1.00	40.67	6
	ATOM	203	CB	LYS A 289	23.655	22.708	41.877	1.00	42.25	6
	ATOM	204	CG	LYS A 289	22.271	22.492	41.247	1.00	39.53	6
	ATOM	205	CD	LYS A 289	22.331	21.606	40.012	1.00	43.19	6
30	ATOM	206	CE	LYS A 289	20.941	21.362	39.447	1.00	45.74	6
	ATOM	207	NZ	LYS A 289	20.273	20.165	40.006	1.00	52.49	7
	ATOM	208	C	LYS A 289	24.948	23.185	44.003	1.00	41.50	6
	ATOM	209	O	LYS A 289	25.642	22.184	44.080	1.00	39.77	8
	ATOM	210	N	LEU A 290	25.312	24.370	44.490	1.00	40.68	7
35	ATOM	211	CA	LEU A 290	26.594	24.583	45.149	1.00	39.33	6
	ATOM	212	CB	LEU A 290	27.153	25.972	44.829	1.00	36.14	6
	ATOM	213	CG	LEU A 290	27.358	26.290	43.365	1.00	34.81	6
	ATOM	214	CD1	LEU A 290	27.945	27.675	43.208	1.00	29.07	6
	ATOM	215	CD2	LEU A 290	28.267	25.242	42.757	1.00	33.45	6
40	ATOM	216	C	LEU A 290	26.434	24.405	46.652	1.00	40.08	6
	ATOM	217	O	LEU A 290	25.803	25.235	47.333	1.00	42.00	8
	ATOM	218	N	PRO A 291	27.028	23.333	47.210	1.00	40.27	7
	ATOM	219	CD	PRO A 291	27.851	22.330	46.519	1.00	39.65	6
	ATOM	220	CA	PRO A 291	26.905	23.096	48.659	1.00	38.28	6
45	ATOM	221	CB	PRO A 291	27.755	21.860	48.911	1.00	35.88	6
	ATOM	222	CG	PRO A 291	28.202	21.355	47.585	1.00	34.19	6
	ATOM	223	C	PRO A 291	27.327	24.298	49.522	1.00	40.05	6
	ATOM	224	O	PRO A 291	26.571	24.739	50.391	1.00	41.33	8
	ATOM	225	N	MET A 292	28.522	24.843	49.299	1.00	40.59	7
50	ATOM	226	CA	MET A 292	29.021	25.957	50.097	1.00	42.86	6
	ATOM	227	CB	MET A 292	30.313	26.475	49.477	1.00	43.28	6
	ATOM	228	CG	MET A 292	31.269	25.378	49.050	1.00	50.35	6
	ATOM	229	SD	MET A 292	32.895	26.096	48.757	1.00	51.17	16
	ATOM	230	CE	MET A 292	33.812	24.647	48.074	1.00	54.63	6
55	ATOM	231	C	MET A 292	27.984	27.066	50.149	1.00	41.05	6
	ATOM	232	O	MET A 292	27.986	27.886	51.057	1.00	39.66	8
	ATOM	233	N	PHE A 293	27.080	27.078	49.172	1.00	39.30	7
	ATOM	234	CA	PHE A 293	26.030	28.091	49.114	1.00	40.92	6

5	ATOM	235	CB	PHE A 293	25.398	28.715	47.524	1.00	40.98	6
	ATOM	236	CG	PHE A 293	24.348	29.168	47.524	1.00	42.78	6
	ATOM	237	CD1	PHE A 293	24.654	30.493	47.747	1.00	44.40	6
	ATOM	238	CD2	PHE A 293	23.071	28.833	47.116	1.00	43.66	6
	ATOM	239	CE1	PHE A 293	23.701	31.478	47.564	1.00	39.83	6
10	ATOM	240	CE2	PHE A 293	22.112	29.819	46.930	1.00	46.21	6
	ATOM	241	CZ	PHE A 293	22.430	31.146	47.155	1.00	45.18	6
	ATOM	242	C	PHE A 293	24.979	27.772	50.164	1.00	45.54	6
	ATOM	243	O	PHE A 293	24.686	28.576	51.034	1.00	42.01	8
	ATOM	244	N	CYS A 294	24.426	26.572	50.062	1.00	47.05	7
15	ATOM	245	CA	CYS A 294	23.386	26.125	50.962	1.00	50.15	6
	ATOM	246	CB	CYS A 294	22.944	24.733	50.524	1.00	45.90	6
	ATOM	247	SG	CYS A 294	22.303	24.663	48.829	1.00	51.50	16
	ATOM	248	C	CYS A 294	23.825	26.125	52.423	1.00	51.38	6
	ATOM	249	O	CYS A 294	23.008	25.954	53.322	1.00	53.83	8
20	ATOM	250	N	GLU A 295	25.119	26.327	52.645	1.00	49.72	7
	ATOM	251	CA	GLU A 295	25.666	26.384	53.996	1.00	52.53	6
	ATOM	252	CB	GLU A 295	27.103	25.830	54.015	1.00	57.40	6
	ATOM	253	CG	GLU A 295	27.182	24.309	54.061	1.00	69.63	6
	ATOM	254	CD	GLU A 295	26.660	23.747	55.342	1.00	78.49	6
25	ATOM	255	OE1	GLU A 295	27.291	23.946	56.412	1.00	82.82	8
	ATOM	256	OE2	GLU A 295	25.590	23.086	55.335	1.00	85.30	8
	ATOM	257	C	GLU A 295	25.653	27.831	54.488	1.00	48.54	6
	ATOM	258	O	GLU A 295	26.365	28.184	55.426	1.00	49.82	8
	ATOM	259	N	LEU A 296	24.804	28.631	53.846	1.00	43.79	7
30	ATOM	260	CA	LEU A 296	24.670	30.034	54.159	1.00	45.42	6
	ATOM	261	CB	LEU A 296	25.062	30.864	52.923	1.00	41.04	6
	ATOM	262	CG	LEU A 296	26.438	30.658	52.315	1.00	42.74	6
	ATOM	263	CD1	LEU A 296	26.447	31.030	50.861	1.00	40.99	6
	ATOM	264	CD2	LEU A 296	27.437	31.454	53.086	1.00	39.44	6
35	ATOM	265	C	LEU A 296	23.239	30.366	54.548	1.00	45.56	6
	ATOM	266	O	LEU A 296	22.301	29.660	54.148	1.00	43.07	8
	ATOM	267	N	PRO A 297	23.050	31.405	55.365	1.00	46.99	7
	ATOM	268	CD	PRO A 297	24.121	32.241	55.930	1.00	47.12	6
	ATOM	269	CA	PRO A 297	21.700	31.811	55.787	1.00	49.61	6
40	ATOM	270	CB	PRO A 297	21.937	32.990	56.738	1.00	49.91	6
	ATOM	271	CG	PRO A 297	23.401	33.155	56.872	1.00	51.28	6
	ATOM	272	C	PRO A 297	20.864	32.212	54.558	1.00	49.59	6
	ATOM	273	O	PRO A 297	21.402	32.684	53.556	1.00	51.66	8
	ATOM	274	N	CYS A 298	19.545	32.035	54.655	1.00	51.02	7
45	ATOM	275	CA	CYS A 298	18.618	32.369	53.567	1.00	52.86	6
	ATOM	276	CB	CYS A 298	17.201	31.877	53.915	1.00	54.57	6
	ATOM	277	SG	CYS A 298	16.040	33.162	54.440	1.00	67.87	16
	ATOM	278	C	CYS A 298	18.583	33.863	53.291	1.00	48.51	6
	ATOM	279	O	CYS A 298	18.039	34.288	52.282	1.00	49.58	8
50	ATOM	280	N	GLU A 299	19.144	34.654	54.202	1.00	44.17	7
	ATOM	281	CA	GLU A 299	19.179	36.096	54.016	1.00	47.57	6
	ATOM	282	CB	GLU A 299	19.265	36.833	55.360	1.00	49.92	6
	ATOM	283	CG	GLU A 299	17.931	36.996	56.125	1.00	59.30	6
	ATOM	284	CD	GLU A 299	17.613	35.904	57.095	1.00	63.80	6
55	ATOM	285	OE1	GLU A 299	16.512	35.952	57.706	1.00	69.03	8
	ATOM	286	OE2	GLU A 299	18.436	34.976	57.292	1.00	67.10	8
	ATOM	287	C	GLU A 299	20.359	36.492	53.152	1.00	46.57	6
	ATOM	288	O	GLU A 299	20.265	37.441	52.379	1.00	44.65	8

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5	ATOM	289	N	ASP A 300	21.467	35.788	52.294	1.00	43.32	7				
	ATOM	290	CA	ASP A 300	22.661	36.042	52.509	1.00	43.32	6				
	ATOM	291	CB	ASP A 300	23.919	35.513	53.213	1.00	37.38	6				
	ATOM	292	CG	ASP A 300	24.223	36.239	54.473	1.00	36.23	6				
	ATOM	293	OD1	ASP A 300	24.153	37.488	54.493	1.00	35.87	8				
10	ATOM	294	OD2	ASP A 300	24.572	35.575	55.483	1.00	40.14	8				
	ATOM	295	C	ASP A 300	22.514	35.390	51.138	1.00	42.81	6				
	ATOM	296	O	ASP A 300	22.775	36.021	50.113	1.00	46.02	8				
	ATOM	297	N	GLN A 301	22.095	34.124	51.137	1.00	38.60	7				
	ATOM	298	CA	GLN A 301	21.896	33.390	49.902	1.00	40.00	6				
15	ATOM	299	CB	GLN A 301	20.991	32.179	50.137	1.00	38.59	6				
	ATOM	300	CG	GLN A 301	21.644	31.003	50.808	1.00	40.26	6				
	ATOM	301	CD	GLN A 301	20.690	29.824	50.988	1.00	44.15	6				
	ATOM	302	OE1	GLN A 301	19.658	29.957	51.675	1.00	45.73	8				
	ATOM	303	NE2	GLN A 301	21.027	28.685	50.394	1.00	46.13	7				
20	ATOM	304	C	GLN A 301	21.242	34.305	48.877	1.00	41.64	6				
	ATOM	305	O	GLN A 301	21.482	34.185	47.686	1.00	45.02	8				
	ATOM	306	N	ILE A 302	20.413	35.228	49.372	1.00	41.01	7				
	ATOM	307	CA	ILE A 302	19.726	36.179	48.511	1.00	40.23	6				
	ATOM	308	CB	ILE A 302	18.502	36.774	49.217	1.00	39.52	6				
25	ATOM	309	CG2	ILE A 302	17.818	37.788	48.342	1.00	31.98	6				
	ATOM	310	CG1	ILE A 302	17.502	35.673	49.581	1.00	40.77	6				
	ATOM	311	CD1	ILE A 302	17.003	34.897	48.385	1.00	45.43	6				
	ATOM	312	C	ILE A 302	20.698	37.268	48.096	1.00	38.58	6				
	ATOM	313	O	ILE A 302	20.960	37.453	46.906	1.00	40.81	8				
30	ATOM	314	N	ILE A 303	21.228	37.972	49.097	1.00	37.50	7				
	ATOM	315	CA	ILE A 303	22.179	39.060	48.874	1.00	39.33	6				
	ATOM	316	CB	ILE A 303	23.023	39.338	50.109	1.00	39.06	6				
	ATOM	317	CG2	ILE A 303	23.946	40.522	49.861	1.00	36.19	6				
	ATOM	318	CG1	ILE A 303	22.141	39.653	51.313	1.00	40.15	6				
35	ATOM	319	CD1	ILE A 303	22.916	39.806	52.589	1.00	36.93	6				
	ATOM	320	C	ILE A 303	23.093	38.705	47.722	1.00	36.49	6				
	ATOM	321	O	ILE A 303	23.354	39.509	46.835	1.00	36.58	8				
	ATOM	322	N	LEU A 304	23.580	37.477	47.762	1.00	32.91	7				
	ATOM	323	CA	LEU A 304	24.465	36.964	46.734	1.00	27.55	6				
40	ATOM	324	CB	LEU A 304	24.935	35.554	47.123	1.00	22.35	6				
	ATOM	325	CG	LEU A 304	26.150	35.480	48.029	1.00	26.88	6				
	ATOM	326	CD1	LEU A 304	26.267	36.731	48.876	1.00	24.82	6				
	ATOM	327	CD2	LEU A 304	26.084	34.226	48.861	1.00	23.69	6				
	ATOM	328	C	LEU A 304	23.764	36.968	45.389	1.00	28.05	6				
45	ATOM	329	O	LEU A 304	24.212	37.623	44.443	1.00	24.68	8				
	ATOM	330	N	LEU A 305	22.657	36.236	45.318	1.00	26.34	7				
	ATOM	331	CA	LEU A 305	21.892	36.147	44.089	1.00	30.91	6				
	ATOM	332	CB	LEU A 305	20.565	35.434	44.359	1.00	32.50	6				
	ATOM	333	CG	LEU A 305	20.637	33.950	44.635	1.00	33.36	6				
50	ATOM	334	CD1	LEU A 305	19.247	33.370	44.779	1.00	33.87	6				
	ATOM	335	CD2	LEU A 305	21.340	33.280	43.466	1.00	31.72	6				
	ATOM	336	C	LEU A 305	21.665	37.524	43.477	1.00	29.76	6				
	ATOM	337	O	LEU A 305	21.954	37.747	42.301	1.00	29.33	8				
	ATOM	338	N	LYS A 306	21.157	38.439	44.298	1.00	29.72	7				
55	ATOM	339	CA	LYS A 306	20.868	39.800	43.864	1.00	34.28	6				
	ATOM	340	CB	LYS A 306	20.293	40.615	45.026	1.00	35.98	6				
	ATOM	341	CG	LYS A 306	18.919	40.163	45.511	1.00	43.35	6				
	ATOM	342	CD	LYS A 306	18.397	41.127	46.559	1.00	51.50	6				



5	ATOM	343	CE	LYS A 306	18.271	42.515	45.971	1.00	53.26	6
	ATOM	344	NZ	LYS A 306	18.325	43.548	47.038	1.00	59.61	7
	ATOM	345	C	LYS A 306	22.075	40.527	43.302	1.00	35.25	6
	ATOM	346	O	LYS A 306	21.972	41.286	42.334	1.00	33.95	8
	ATOM	347	N	GLY A 307	23.228	40.306	43.928	1.00	35.79	7
10	ATOM	348	CA	GLY A 307	24.445	40.962	43.482	1.00	34.59	6
	ATOM	349	C	GLY A 307	25.109	40.353	42.259	1.00	33.80	6
	ATOM	350	O	GLY A 307	25.489	41.087	41.344	1.00	31.59	8
	ATOM	351	N	CYS A 308	25.248	39.024	42.256	1.00	31.15	7
	ATOM	352	CA	CYS A 308	25.899	38.326	41.174	1.00	29.04	6
15	ATOM	353	CB	CYS A 308	26.604	37.089	41.704	1.00	27.59	6
	ATOM	354	SG	CYS A 308	25.472	35.770	42.071	1.00	30.50	16
	ATOM	355	C	CYS A 308	24.974	37.870	40.062	1.00	30.59	6
	ATOM	356	O	CYS A 308	25.458	37.319	39.077	1.00	33.77	8
	ATOM	357	N	CYS A 309	23.664	38.084	40.195	1.00	28.46	7
20	ATOM	358	CA	CYS A 309	22.739	37.623	39.168	1.00	30.10	6
	ATOM	359	CB	CYS A 309	21.311	38.004	39.490	1.00	33.43	6
	ATOM	360	SG	CYS A 309	20.198	37.299	38.307	1.00	35.20	16
	ATOM	361	C	CYS A 309	23.065	38.123	37.788	1.00	27.72	6
	ATOM	362	O	CYS A 309	23.212	37.334	36.865	1.00	27.69	8
25	ATOM	363	N	MET A 310	23.157	39.439	37.639	1.00	26.15	7
	ATOM	364	CA	MET A 310	23.476	40.016	36.342	1.00	26.06	6
	ATOM	365	CB	MET A 310	23.482	41.547	36.419	1.00	25.32	6
	ATOM	366	CG	MET A 310	23.913	42.230	35.109	1.00	24.08	6
	ATOM	367	SD	MET A 310	22.765	41.751	33.762	1.00	27.71	16
30	ATOM	368	CE	MET A 310	23.650	42.321	32.270	1.00	28.50	6
	ATOM	369	C	MET A 310	24.842	39.527	35.908	1.00	25.94	6
	ATOM	370	O	MET A 310	25.020	39.076	34.788	1.00	28.09	8
	ATOM	371	N	GLU A 311	25.800	39.638	36.826	1.00	25.39	7
	ATOM	372	CA	GLU A 311	27.176	39.234	36.589	1.00	27.03	6
35	ATOM	373	CB	GLU A 311	27.973	39.303	37.900	1.00	24.39	6
	ATOM	374	CG	GLU A 311	27.842	40.628	38.668	1.00	26.00	6
	ATOM	375	CD	GLU A 311	28.726	40.720	39.870	1.00	23.95	6
	ATOM	376	OE1	GLU A 311	28.891	39.706	40.588	1.00	19.72	8
	ATOM	377	OE2	GLU A 311	29.270	41.818	40.159	1.00	26.51	8
40	ATOM	378	C	GLU A 311	27.266	37.827	35.997	1.00	27.51	6
	ATOM	379	O	GLU A 311	27.956	37.620	35.014	1.00	29.67	8
	ATOM	380	N	ILE A 312	26.569	36.866	36.602	1.00	26.82	7
	ATOM	381	CA	ILE A 312	26.593	35.497	36.112	1.00	25.71	6
	ATOM	382	CB	ILE A 312	25.991	34.518	37.123	1.00	23.35	6
45	ATOM	383	CG2	ILE A 312	25.917	33.123	36.533	1.00	20.27	6
	ATOM	384	CG1	ILE A 312	26.837	34.471	38.398	1.00	20.88	6
	ATOM	385	CD1	ILE A 312	26.462	33.342	39.341	1.00	18.15	6
	ATOM	386	C	ILE A 312	25.871	35.371	34.791	1.00	27.91	6
	ATOM	387	O	ILE A 312	26.274	34.593	33.934	1.00	28.96	8
50	ATOM	388	N	MET A 313	24.788	36.130	34.633	1.00	27.66	7
	ATOM	389	CA	MET A 313	24.013	36.081	33.395	1.00	30.18	6
	ATOM	390	CB	MET A 313	22.716	36.888	33.508	1.00	36.89	6
	ATOM	391	CG	MET A 313	21.608	36.198	34.305	1.00	37.95	6
	ATOM	392	SD	MET A 313	19.892	36.817	34.055	1.00	42.38	16
55	ATOM	393	CE	MET A 313	20.034	38.503	34.740	1.00	40.68	6
	ATOM	394	C	MET A 313	24.834	36.579	32.222	1.00	27.43	6
	ATOM	395	O	MET A 313	25.116	35.814	31.308	1.00	28.61	8
	ATOM	396	N	SER A 314	25.209	37.859	32.253	1.00	24.88	7

5	ATOM	397	CA	SER	A	314	26.005	38.472	31.197	1.00	27.98	6
	ATOM	398	CB	SER	A	314	26.354	39.914	31.581	1.00	29.64	6
	ATOM	399	OG	SER	A	314	26.956	39.972	32.858	1.00	43.44	8
	ATOM	400	C	SER	A	314	27.275	37.679	30.851	1.00	22.30	6
	ATOM	401	O	SER	A	314	27.675	37.629	29.690	1.00	24.18	8
10	ATOM	402	N	LEU	A	315	27.905	37.048	31.845	1.00	23.99	7
	ATOM	403	CA	LEU	A	315	29.099	36.261	31.563	1.00	25.07	6
	ATOM	404	CB	LEU	A	315	29.685	35.593	32.816	1.00	19.11	6
	ATOM	405	CG	LEU	A	315	30.675	34.479	32.505	1.00	20.39	6
	ATOM	406	CD1	LEU	A	315	31.866	35.040	31.756	1.00	18.92	6
15	ATOM	407	CD2	LEU	A	315	31.125	33.789	33.765	1.00	12.93	6
	ATOM	408	C	LEU	A	315	28.700	35.180	30.597	1.00	24.53	6
	ATOM	409	O	LEU	A	315	29.304	35.036	29.556	1.00	26.32	8
	ATOM	410	N	ARG	A	316	27.678	34.426	30.982	1.00	28.18	7
	ATOM	411	CA	ARG	A	316	27.151	33.312	30.216	1.00	27.54	6
20	ATOM	412	CB	ARG	A	316	25.915	32.752	30.928	1.00	27.39	6
	ATOM	413	CG	ARG	A	316	26.188	32.190	32.336	1.00	22.00	6
	ATOM	414	CD	ARG	A	316	24.934	31.526	32.901	1.00	18.78	6
	ATOM	415	NE	ARG	A	316	25.245	30.376	33.721	1.00	26.57	7
	ATOM	416	CZ	ARG	A	316	24.341	29.468	34.054	1.00	30.81	6
25	ATOM	417	NH1	ARG	A	316	23.084	29.614	33.639	1.00	33.71	7
	ATOM	418	NH2	ARG	A	316	24.701	28.416	34.776	1.00	33.13	7
	ATOM	419	C	ARG	A	316	26.774	33.660	28.794	1.00	28.09	6
	ATOM	420	O	ARG	A	316	26.737	32.792	27.931	1.00	32.41	8
	ATOM	421	N	ALA	A	317	26.484	34.936	28.571	1.00	28.36	7
30	ATOM	422	CA	ALA	A	317	26.094	35.411	27.264	1.00	26.64	6
	ATOM	423	CB	ALA	A	317	25.232	36.666	27.418	1.00	22.93	6
	ATOM	424	C	ALA	A	317	27.323	35.714	26.417	1.00	28.35	6
	ATOM	425	O	ALA	A	317	27.398	35.342	25.252	1.00	32.10	8
	ATOM	426	N	ALA	A	318	28.286	36.396	27.026	1.00	29.12	7
35	ATOM	427	CA	ALA	A	318	29.515	36.760	26.350	1.00	27.50	6
	ATOM	428	CB	ALA	A	318	30.434	37.452	27.333	1.00	28.39	6
	ATOM	429	C	ALA	A	318	30.181	35.502	25.825	1.00	28.10	6
	ATOM	430	O	ALA	A	318	30.600	35.447	24.678	1.00	28.18	8
	ATOM	431	N	VAL	A	319	30.255	34.491	26.700	1.00	29.16	7
40	ATOM	432	CA	VAL	A	319	30.880	33.198	26.393	1.00	35.24	6
	ATOM	433	CB	VAL	A	319	30.703	32.210	27.547	1.00	27.34	6
	ATOM	434	CG1	VAL	A	319	30.895	32.891	28.858	1.00	29.96	6
	ATOM	435	CG2	VAL	A	319	29.353	31.552	27.482	1.00	31.70	6
	ATOM	436	C	VAL	A	319	30.215	32.608	25.165	1.00	40.01	6
45	ATOM	437	O	VAL	A	319	30.640	31.575	24.680	1.00	42.70	8
	ATOM	438	N	ARG	A	320	29.176	33.284	24.683	1.00	38.64	7
	ATOM	439	CA	ARG	A	320	28.415	32.822	23.545	1.00	38.61	6
	ATOM	440	CB	ARG	A	320	27.031	32.458	24.043	1.00	37.26	6
	ATOM	441	CG	ARG	A	320	26.863	30.991	24.192	1.00	43.12	6
50	ATOM	442	CD	ARG	A	320	25.637	30.642	25.014	1.00	50.79	6
	ATOM	443	NE	ARG	A	320	25.258	29.256	24.770	1.00	54.71	7
	ATOM	444	CZ	ARG	A	320	24.331	28.625	25.501	1.00	57.89	6
	ATOM	445	NH1	ARG	A	320	23.667	29.291	26.440	1.00	49.08	7
	ATOM	446	NH2	ARG	A	320	23.964	27.385	25.242	1.00	59.59	7
55	ATOM	447	C	ARG	A	320	28.292	33.825	22.405	1.00	42.14	6
	ATOM	448	O	ARG	A	320	27.251	33.909	21.748	1.00	46.30	8
	ATOM	449	N	TYR	A	321	29.352	34.583	22.173	1.00	42.04	7
	ATOM	450	CA	TYR	A	321	29.366	35.555	21.098	1.00	42.70	6

5	ATOM	451	CB	TYR	A	321	30.083	36.810	21.575	1.00	38.01	6
	ATOM	452	CG	TYR	A	321	30.601	37.650	20.448	1.00	37.94	6
	ATOM	453	CD1	TYR	A	321	29.733	38.296	19.574	1.00	33.85	6
	ATOM	454	CE1	TYR	A	321	30.235	39.037	18.494	1.00	34.49	6
	ATOM	455	CD2	TYR	A	321	31.966	37.743	20.224	1.00	28.03	6
10	ATOM	456	CE2	TYR	A	321	32.473	38.475	19.153	1.00	32.69	6
	ATOM	457	CZ	TYR	A	321	31.612	39.125	18.276	1.00	35.18	6
	ATOM	458	OH	TYR	A	321	32.107	39.866	17.223	1.00	39.48	8
	ATOM	459	C	TYR	A	321	30.085	35.005	19.877	1.00	45.51	6
	ATOM	460	O	TYR	A	321	31.261	34.697	19.951	1.00	48.02	8
15	ATOM	461	N	ASP	A	322	29.354	34.879	18.773	1.00	44.56	7
	ATOM	462	CA	ASP	A	322	29.912	34.400	17.502	1.00	45.86	6
	ATOM	463	CB	ASP	A	322	28.804	33.670	16.736	1.00	46.64	6
	ATOM	464	CG	ASP	A	322	29.050	33.608	15.255	1.00	40.00	6
	ATOM	465	OD1	ASP	A	322	30.010	34.256	14.768	1.00	40.00	8
20	ATOM	466	OD2	ASP	A	322	28.262	32.929	14.536	1.00	40.00	8
	ATOM	467	C	ASP	A	322	30.460	35.629	16.755	1.00	45.82	6
	ATOM	468	O	ASP	A	322	29.678	36.464	16.271	1.00	45.38	8
	ATOM	469	N	PRO	A	323	31.800	35.735	16.584	1.00	46.53	7
	ATOM	470	CD	PRO	A	323	32.774	34.719	16.991	1.00	47.16	6
25	ATOM	471	CA	PRO	A	323	32.424	36.889	15.890	1.00	46.63	6
	ATOM	472	CB	PRO	A	323	33.921	36.603	15.936	1.00	43.95	6
	ATOM	473	CG	PRO	A	323	34.099	35.303	16.582	1.00	43.93	6
	ATOM	474	C	PRO	A	323	31.953	37.087	14.453	1.00	48.34	6
	ATOM	475	O	PRO	A	323	31.797	38.210	13.960	1.00	50.84	8
30	ATOM	476	N	GLU	A	324	31.778	35.970	13.752	1.00	52.39	7
	ATOM	477	CA	GLU	A	324	31.339	35.968	12.370	1.00	55.85	6
	ATOM	478	CB	GLU	A	324	31.035	34.528	11.965	1.00	55.54	6
	ATOM	479	CG	GLU	A	324	32.224	33.584	12.104	1.00	40.00	6
	ATOM	480	CD	GLU	A	324	33.432	34.023	11.310	1.00	40.00	6
35	ATOM	481	OE1	GLU	A	324	33.350	35.040	10.555	1.00	40.00	8
	ATOM	482	OE2	GLU	A	324	34.506	33.356	11.415	1.00	40.00	8
	ATOM	483	C	GLU	A	324	30.077	36.798	12.277	1.00	54.94	6
	ATOM	484	O	GLU	A	324	30.070	37.892	11.730	1.00	59.81	8
	ATOM	485	N	SER	A	325	29.009	36.212	12.810	1.00	52.95	7
40	ATOM	486	CA	SER	A	325	27.695	36.812	12.839	1.00	50.10	6
	ATOM	487	CB	SER	A	325	26.701	35.797	13.402	1.00	48.23	6
	ATOM	488	OG	SER	A	325	27.183	35.239	14.615	1.00	48.71	8
	ATOM	489	C	SER	A	325	27.651	38.093	13.659	1.00	50.61	6
	ATOM	490	O	SER	A	325	26.885	38.992	13.354	1.00	52.19	8
45	ATOM	491	N	GLU	A	326	28.495	38.168	14.687	1.00	45.64	7
	ATOM	492	CA	GLU	A	326	28.567	39.341	15.546	1.00	43.35	6
	ATOM	493	CB	GLU	A	326	28.830	40.608	14.711	1.00	42.74	6
	ATOM	494	CG	GLU	A	326	30.148	40.606	13.945	1.00	50.32	6
	ATOM	495	CD	GLU	A	326	30.451	41.925	13.313	1.00	56.34	6
50	ATOM	496	OE1	GLU	A	326	31.509	42.046	12.649	1.00	59.31	8
	ATOM	497	OE2	GLU	A	326	29.656	42.890	13.452	1.00	55.74	8
	ATOM	498	C	GLU	A	326	27.288	39.526	16.340	1.00	40.23	6
	ATOM	499	O	GLU	A	326	26.695	40.603	16.340	1.00	40.44	8
	ATOM	500	N	THR	A	327	26.888	38.474	17.051	1.00	35.90	7
55	ATOM	501	CA	THR	A	327	25.663	38.506	17.860	1.00	37.29	6
	ATOM	502	CB	THR	A	327	24.466	38.057	17.024	1.00	37.63	6
	ATOM	503	OG1	THR	A	327	24.661	36.709	16.580	1.00	38.12	8
	ATOM	504	CG2	THR	A	327	24.269	38.965	15.810	1.00	39.90	6

5	ATOM	505	C	THR	A	327	25.767	37.562	19.038	1.00	39.49	6
	ATOM	506	O	THR	A	327	26.284	36.458	18.903	1.00	40.50	8
	ATOM	507	N	LEU	A	328	25.250	37.987	20.184	1.00	36.64	7
	ATOM	508	CA	LEU	A	328	25.264	37.141	21.381	1.00	37.73	6
	ATOM	509	CB	LEU	A	328	25.148	37.999	22.650	1.00	37.78	6
10	ATOM	510	CG	LEU	A	328	26.102	39.150	22.843	1.00	36.26	6
	ATOM	511	CD1	LEU	A	328	26.066	39.623	24.272	1.00	36.56	6
	ATOM	512	CD2	LEU	A	328	27.481	38.688	22.500	1.00	39.85	6
	ATOM	513	C	LEU	A	328	24.063	36.220	21.244	1.00	37.27	6
	ATOM	514	O	LEU	A	328	23.306	36.337	20.279	1.00	34.96	8
15	ATOM	515	N	THR	A	329	23.891	35.317	22.205	1.00	39.73	7
	ATOM	516	CA	THR	A	329	22.785	34.376	22.180	1.00	40.81	6
	ATOM	517	CB	THR	A	329	23.241	32.991	21.699	1.00	42.67	6
	ATOM	518	OG1	THR	A	329	23.879	33.103	20.421	1.00	42.52	8
	ATOM	519	CG2	THR	A	329	22.026	32.057	21.589	1.00	43.52	6
20	ATOM	520	C	THR	A	329	22.168	34.245	23.548	1.00	44.31	6
	ATOM	521	O	THR	A	329	22.526	33.370	24.320	1.00	43.72	8
	ATOM	522	N	LEU	A	330	21.237	35.149	23.830	1.00	44.62	7
	ATOM	523	CA	LEU	A	330	20.532	35.170	25.111	1.00	45.09	6
	ATOM	524	CB	LEU	A	330	19.677	36.444	25.195	1.00	44.66	6
25	ATOM	525	CG	LEU	A	330	20.436	37.750	25.259	1.00	51.06	6
	ATOM	526	CD1	LEU	A	330	21.405	37.831	24.104	1.00	48.58	6
	ATOM	527	CD2	LEU	A	330	19.466	38.909	25.238	1.00	45.18	6
	ATOM	528	C	LEU	A	330	19.656	33.919	25.301	1.00	48.06	6
	ATOM	529	O	LEU	A	330	19.049	33.422	24.359	1.00	49.33	8
30	ATOM	530	N	ASN	A	331	19.618	33.431	26.540	1.00	52.20	7
	ATOM	531	CA	ASN	A	331	18.842	32.256	26.913	1.00	54.41	6
	ATOM	532	CB	ASN	A	331	17.361	32.628	27.009	1.00	54.94	6
	ATOM	533	CG	ASN	A	331	16.724	32.112	28.269	1.00	60.35	6
	ATOM	534	OD1	ASN	A	331	17.124	32.505	29.383	1.00	61.84	8
35	ATOM	535	ND2	ASN	A	331	15.750	31.238	28.117	1.00	65.92	7
	ATOM	536	C	ASN	A	331	19.016	31.108	25.934	1.00	58.00	6
	ATOM	537	O	ASN	A	331	18.243	30.157	25.941	1.00	60.17	8
	ATOM	538	N	GLY	A	332	20.063	31.196	25.114	1.00	58.45	7
	ATOM	539	CA	GLY	A	332	20.341	30.161	24.131	1.00	58.55	6
40	ATOM	540	C	GLY	A	332	19.316	30.016	23.021	1.00	59.79	6
	ATOM	541	O	GLY	A	332	19.413	29.094	22.213	1.00	61.32	8
	ATOM	542	N	GLU	A	333	18.346	30.929	22.983	1.00	60.28	7
	ATOM	543	CA	GLU	A	333	17.294	30.883	21.985	1.00	59.13	6
	ATOM	544	CB	GLU	A	333	15.919	30.875	22.662	1.00	62.40	6
45	ATOM	545	CG	GLU	A	333	15.667	29.750	23.658	1.00	75.69	6
	ATOM	546	CD	GLU	A	333	14.341	29.865	24.346	1.00	80.41	6
	ATOM	547	OE1	GLU	A	333	14.052	30.932	24.945	1.00	79.98	8
	ATOM	548	OE2	GLU	A	333	13.549	28.884	24.329	1.00	83.81	8
	ATOM	549	C	GLU	A	333	17.356	32.090	21.073	1.00	57.18	6
50	ATOM	550	O	GLU	A	333	17.239	31.969	19.852	1.00	57.50	8
	ATOM	551	N	MET	A	334	17.512	33.258	21.696	1.00	55.20	7
	ATOM	552	CA	MET	A	334	17.561	34.529	20.980	1.00	50.85	6
	ATOM	553	CB	MET	A	334	16.751	35.556	21.763	1.00	48.70	6
	ATOM	554	CG	MET	A	334	16.859	36.947	21.212	1.00	45.39	6
55	ATOM	555	SD	MET	A	334	15.881	38.186	22.127	1.00	44.56	16
	ATOM	556	CE	MET	A	334	14.229	37.371	22.113	1.00	45.25	6
	ATOM	557	C	MET	A	334	18.956	35.087	20.713	1.00	51.59	6
	ATOM	558	O	MET	A	334	19.739	35.268	21.633	1.00	52.52	8

5	ATOM	559	N	ALA	A	335	19.234	35.371	19.444	1.00	51.00	7
	ATOM	560	CA	ALA	A	335	20.520	35.932	19.039	1.00	48.98	6
	ATOM	561	CB	ALA	A	335	20.997	35.254	17.768	1.00	47.86	6
	ATOM	562	C	ALA	A	335	20.342	37.420	18.805	1.00	51.01	6
	ATOM	563	O	ALA	A	335	19.594	37.830	17.919	1.00	51.61	8
10	ATOM	564	N	VAL	A	336	21.024	38.232	19.612	1.00	46.62	7
	ATOM	565	CA	VAL	A	336	20.910	39.699	19.502	1.00	42.35	6
	ATOM	566	CB	VAL	A	336	20.517	40.325	20.840	1.00	42.41	6
	ATOM	567	CG1	VAL	A	336	19.242	39.691	21.361	1.00	42.00	6
	ATOM	568	CG2	VAL	A	336	21.639	40.211	21.852	1.00	40.32	6
15	ATOM	569	C	VAL	A	336	22.204	40.321	19.036	1.00	45.33	6
	ATOM	570	O	VAL	A	336	23.263	39.691	19.025	1.00	47.42	8
	ATOM	571	N	THR	A	337	22.090	41.590	18.668	1.00	41.60	7
	ATOM	572	CA	THR	A	337	23.230	42.377	18.175	1.00	39.69	6
	ATOM	573	CB	THR	A	337	22.882	43.061	16.852	1.00	41.35	6
20	ATOM	574	OG1	THR	A	337	21.987	44.157	17.080	1.00	49.35	8
	ATOM	575	CG2	THR	A	337	22.216	42.067	15.904	1.00	40.38	6
	ATOM	576	C	THR	A	337	23.588	43.481	19.159	1.00	37.88	6
	ATOM	577	O	THR	A	337	22.734	43.989	19.892	1.00	34.06	8
	ATOM	578	N	ARG	A	338	24.865	43.849	19.138	1.00	37.61	7
25	ATOM	579	CA	ARG	A	338	25.388	44.919	19.984	1.00	38.68	6
	ATOM	580	CB	ARG	A	338	26.669	45.479	19.351	1.00	35.95	6
	ATOM	581	CG	ARG	A	338	27.250	46.713	20.038	1.00	38.83	6
	ATOM	582	CD	ARG	A	338	28.443	47.254	19.247	1.00	35.88	6
	ATOM	583	NE	ARG	A	338	29.559	46.320	19.175	1.00	37.42	7
30	ATOM	584	CZ	ARG	A	338	30.449	46.122	20.145	1.00	30.20	6
	ATOM	585	NH1	ARG	A	338	30.338	46.791	21.295	1.00	27.98	7
	ATOM	586	NH2	ARG	A	338	31.433	45.240	19.954	1.00	27.40	7
	ATOM	587	C	ARG	A	338	24.333	46.010	20.085	1.00	38.09	6
	ATOM	588	O	ARG	A	338	23.894	46.397	21.169	1.00	34.12	8
35	ATOM	589	N	GLY	A	339	23.915	46.496	18.922	1.00	41.25	7
	ATOM	590	CA	GLY	A	339	22.918	47.547	18.890	1.00	41.35	6
	ATOM	591	C	GLY	A	339	21.692	47.140	19.672	1.00	41.23	6
	ATOM	592	O	GLY	A	339	21.445	47.671	20.750	1.00	38.30	8
	ATOM	593	N	GLN	A	340	20.924	46.203	19.105	1.00	38.58	7
40	ATOM	594	CA	GLN	A	340	19.701	45.700	19.729	1.00	40.79	6
	ATOM	595	CB	GLN	A	340	19.436	44.260	19.253	1.00	40.82	6
	ATOM	596	CG	GLN	A	340	19.087	44.146	17.767	1.00	41.10	6
	ATOM	597	CD	GLN	A	340	18.876	42.705	17.305	1.00	48.84	6
	ATOM	598	OE1	GLN	A	340	19.826	41.888	17.309	1.00	50.53	8
45	ATOM	599	NE2	GLN	A	340	17.650	42.393	16.907	1.00	54.25	7
	ATOM	600	C	GLN	A	340	19.779	45.750	21.263	1.00	41.50	6
	ATOM	601	O	GLN	A	340	18.998	46.444	21.923	1.00	42.72	8
	ATOM	602	N	LEU	A	341	20.758	45.026	21.806	1.00	42.00	7
	ATOM	603	CA	LEU	A	341	20.952	44.947	23.243	1.00	38.10	6
50	ATOM	604	CB	LEU	A	341	22.209	44.145	23.575	1.00	36.66	6
	ATOM	605	CG	LEU	A	341	22.361	43.804	25.029	1.00	39.94	6
	ATOM	606	CD1	LEU	A	341	21.219	42.884	25.410	1.00	34.98	6
	ATOM	607	CD2	LEU	A	341	23.685	43.128	25.284	1.00	40.95	6
	ATOM	608	C	LEU	A	341	21.072	46.321	23.860	1.00	36.37	6
55	ATOM	609	O	LEU	A	341	20.484	46.588	24.892	1.00	37.89	8
	ATOM	610	N	LYS	A	342	21.848	47.184	23.209	1.00	33.29	7
	ATOM	611	CA	LYS	A	342	22.089	48.546	23.679	1.00	35.17	6
	ATOM	612	CB	LYS	A	342	23.057	49.242	22.721	1.00	34.97	6

5	ATOM	613	CG	LYS	A	342	23.655	50.536	23.240	1.00	40.00	6
	ATOM	614	CD	LYS	A	342	24.673	51.109	22.245	1.00	34.48	6
	ATOM	615	CE	LYS	A	342	25.514	52.229	22.873	1.00	37.54	6
	ATOM	616	NZ	LYS	A	342	26.655	52.634	21.987	1.00	42.32	7
	ATOM	617	C	LYS	A	342	20.796	49.349	23.774	1.00	38.29	8
10	ATOM	618	O	LYS	A	342	20.345	49.711	24.861	1.00	36.23	8
	ATOM	619	N	ASN	A	343	20.223	49.622	22.603	1.00	39.25	7
	ATOM	620	CA	ASN	A	343	18.993	50.385	22.485	1.00	40.19	6
	ATOM	621	CB	ASN	A	343	18.521	50.373	21.033	1.00	37.96	6
	ATOM	622	CG	ASN	A	343	19.664	50.550	20.052	1.00	39.22	6
15	ATOM	623	OD1	ASN	A	343	20.428	51.537	20.125	1.00	42.37	8
	ATOM	624	ND2	ASN	A	343	19.773	49.612	19.125	1.00	42.19	7
	ATOM	625	C	ASN	A	343	17.928	49.748	23.375	1.00	40.12	6
	ATOM	626	O	ASN	A	343	17.010	50.417	23.859	1.00	36.01	8
	ATOM	627	N	GLY	A	344	18.073	48.433	23.568	1.00	40.95	7
20	ATOM	628	CA	GLY	A	344	17.152	47.670	24.394	1.00	39.25	6
	ATOM	629	C	GLY	A	344	17.039	48.092	25.842	1.00	38.26	6
	ATOM	630	O	GLY	A	344	16.072	47.724	26.512	1.00	35.69	8
	ATOM	631	N	GLY	A	345	18.017	48.857	26.329	1.00	35.89	7
	ATOM	632	CA	GLY	A	345	17.964	49.301	27.706	1.00	34.00	6
25	ATOM	633	C	GLY	A	345	19.273	49.199	28.443	1.00	38.64	6
	ATOM	634	O	GLY	A	345	19.469	49.888	29.441	1.00	38.14	8
	ATOM	635	N	LEU	A	346	20.170	48.337	27.973	1.00	39.52	7
	ATOM	636	CA	LEU	A	346	21.444	48.180	28.649	1.00	36.05	6
	ATOM	637	CB	LEU	A	346	22.124	46.876	28.209	1.00	35.72	6
30	ATOM	638	CG	LEU	A	346	21.355	45.617	28.501	1.00	34.89	6
	ATOM	639	CD1	LEU	A	346	22.295	44.413	28.422	1.00	44.09	6
	ATOM	640	CD2	LEU	A	346	20.786	45.721	29.902	1.00	34.84	6
	ATOM	641	C	LEU	A	346	22.358	49.361	28.396	1.00	33.52	6
	ATOM	642	O	LEU	A	346	23.267	49.653	29.178	1.00	35.58	8
35	ATOM	643	N	GLY	A	347	22.087	50.056	27.295	1.00	30.47	7
	ATOM	644	CA	GLY	A	347	22.909	51.192	26.931	1.00	33.01	6
	ATOM	645	C	GLY	A	347	24.360	50.768	26.747	1.00	30.72	6
	ATOM	646	O	GLY	A	347	24.669	49.775	26.082	1.00	30.89	8
	ATOM	647	N	VAL	A	348	25.244	51.556	27.355	1.00	31.30	7
40	ATOM	648	CA	VAL	A	348	26.671	51.325	27.286	1.00	31.27	6
	ATOM	649	CB	VAL	A	348	27.441	52.294	28.184	1.00	31.66	6
	ATOM	650	CG1	VAL	A	348	27.067	52.107	29.631	1.00	20.19	6
	ATOM	651	CG2	VAL	A	348	28.931	52.138	27.986	1.00	24.77	6
	ATOM	652	C	VAL	A	348	27.063	49.892	27.678	1.00	33.84	6
45	ATOM	653	O	VAL	A	348	28.095	49.392	27.225	1.00	29.99	8
	ATOM	654	N	VAL	A	349	26.253	49.227	28.514	1.00	33.31	7
	ATOM	655	CA	VAL	A	349	26.568	47.881	28.906	1.00	32.23	6
	ATOM	656	CB	VAL	A	349	25.581	47.259	29.858	1.00	32.59	6
	ATOM	657	CG1	VAL	A	349	25.865	45.795	29.985	1.00	33.68	6
50	ATOM	658	CG2	VAL	A	349	25.687	47.899	31.213	1.00	32.30	6
	ATOM	659	C	VAL	A	349	26.706	46.985	27.726	1.00	34.91	6
	ATOM	660	O	VAL	A	349	27.583	46.136	27.735	1.00	33.73	8
	ATOM	661	N	SER	A	350	25.875	47.134	26.702	1.00	32.81	7
	ATOM	662	CA	SER	A	350	26.001	46.252	25.556	1.00	30.10	6
55	ATOM	663	CB	SER	A	350	25.119	46.665	24.411	1.00	24.95	6
	ATOM	664	OG	SER	A	350	25.209	45.675	23.394	1.00	23.16	8
	ATOM	665	C	SER	A	350	27.445	46.257	25.129	1.00	31.59	6
	ATOM	666	O	SER	A	350	28.116	45.244	25.284	1.00	37.62	8

5	ATOM	667	N	ASP	A	351	27.945	47.367	24.591	1.00	28.60	7
	ATOM	668	CA	ASP	A	351	29.351	47.437	24.183	1.00	29.82	6
	ATOM	669	CB	ASP	A	351	29.808	48.891	24.105	1.00	27.49	6
	ATOM	670	CG	ASP	A	351	28.875	49.744	23.303	1.00	30.22	6
	ATOM	671	OD1	ASP	A	351	28.055	50.483	23.909	1.00	32.61	8
10	ATOM	672	OD2	ASP	A	351	28.942	49.714	22.044	1.00	30.02	8
	ATOM	673	C	ASP	A	351	30.173	46.653	25.231	1.00	30.63	6
	ATOM	674	O	ASP	A	351	30.981	45.792	24.903	1.00	29.54	8
	ATOM	675	N	ALA	A	352	29.939	46.949	26.503	1.00	25.33	7
	ATOM	676	CA	ALA	A	352	30.623	46.280	27.602	1.00	28.59	6
15	ATOM	677	CB	ALA	A	352	30.072	46.799	28.922	1.00	20.95	6
	ATOM	678	C	ALA	A	352	30.492	44.756	27.527	1.00	29.69	6
	ATOM	679	O	ALA	A	352	31.481	44.054	27.587	1.00	30.36	8
	ATOM	680	N	ILE	A	353	29.260	44.260	27.413	1.00	27.63	7
	ATOM	681	CA	ILE	A	353	29.003	42.832	27.326	1.00	27.55	6
20	ATOM	682	CB	ILE	A	353	27.512	42.528	27.429	1.00	28.04	6
	ATOM	683	CG2	ILE	A	353	27.269	41.042	27.289	1.00	23.68	6
	ATOM	684	CG1	ILE	A	353	26.955	42.965	28.789	1.00	27.33	6
	ATOM	685	CD1	ILE	A	353	25.452	42.688	28.944	1.00	26.23	6
	ATOM	686	C	ILE	A	353	29.534	42.207	26.054	1.00	30.88	6
25	ATOM	687	O	ILE	A	353	30.007	41.076	26.068	1.00	31.22	8
	ATOM	688	N	PHE	A	354	29.426	42.917	24.939	1.00	29.86	7
	ATOM	689	CA	PHE	A	354	29.922	42.369	23.686	1.00	31.08	6
	ATOM	690	CB	PHE	A	354	29.371	43.146	22.487	1.00	28.80	6
	ATOM	691	CG	PHE	A	354	28.029	42.643	21.988	1.00	28.80	6
30	ATOM	692	CD1	PHE	A	354	26.872	42.842	22.724	1.00	30.96	6
	ATOM	693	CD2	PHE	A	354	27.950	41.953	20.783	1.00	29.45	6
	ATOM	694	CE1	PHE	A	354	25.657	42.360	22.250	1.00	27.12	6
	ATOM	695	CE2	PHE	A	354	26.738	41.470	20.305	1.00	25.19	6
	ATOM	696	CZ	PHE	A	354	25.590	41.672	21.038	1.00	28.09	6
35	ATOM	697	C	PHE	A	354	31.444	42.399	23.682	1.00	29.17	6
	ATOM	698	O	PHE	A	354	32.087	41.389	23.398	1.00	32.62	8
	ATOM	699	N	ASP	A	355	32.013	43.569	23.980	1.00	23.86	7
	ATOM	700	CA	ASP	A	355	33.466	43.739	24.030	1.00	25.34	6
	ATOM	701	CB	ASP	A	355	33.820	45.053	24.737	1.00	21.41	6
40	ATOM	702	CG	ASP	A	355	33.841	46.226	23.809	1.00	32.08	6
	ATOM	703	OD1	ASP	A	355	32.979	46.322	22.902	1.00	33.58	8
	ATOM	704	OD2	ASP	A	355	34.711	47.117	23.968	1.00	33.20	8
	ATOM	705	C	ASP	A	355	34.074	42.559	24.781	1.00	27.86	6
	ATOM	706	O	ASP	A	355	35.131	42.053	24.410	1.00	32.42	8
45	ATOM	707	N	LEU	A	356	33.387	42.128	25.843	1.00	26.84	7
	ATOM	708	CA	LEU	A	356	33.845	40.993	26.642	1.00	28.66	6
	ATOM	709	CB	LEU	A	356	32.893	40.747	27.825	1.00	25.37	6
	ATOM	710	CG	LEU	A	356	33.235	39.608	28.755	1.00	27.61	6
	ATOM	711	CD1	LEU	A	356	34.538	39.917	29.451	1.00	25.43	6
50	ATOM	712	CD2	LEU	A	356	32.149	39.414	29.765	1.00	27.49	6
	ATOM	713	C	LEU	A	356	33.849	39.779	25.723	1.00	30.44	6
	ATOM	714	O	LEU	A	356	34.884	39.160	25.470	1.00	31.55	8
	ATOM	715	N	GLY	A	357	32.661	39.451	25.218	1.00	32.69	7
	ATOM	716	CA	GLY	A	357	32.511	38.304	24.338	1.00	29.87	6
55	ATOM	717	C	GLY	A	357	33.653	38.157	23.359	1.00	33.12	6
	ATOM	718	O	GLY	A	357	34.302	37.110	23.323	1.00	29.41	8
	ATOM	719	N	MET	A	358	33.876	39.206	22.564	1.00	33.31	7
	ATOM	720	CA	MET	A	358	34.949	39.206	21.580	1.00	35.87	6

5	ATOM	721	CB	MET A 358	35.143	40.663	20.290	1.00	34.56	6
	ATOM	722	CG	MET A 358	33.949	41.145	20.290	1.00	46.43	6
	ATOM	723	SD	MET A 358	34.207	42.776	19.514	1.00	42.13	16
	ATOM	724	CE	MET A 358	34.507	43.855	20.994	1.00	44.29	6
	ATOM	725	C	MET A 358	36.256	38.762	22.230	1.00	33.26	6
10	ATOM	726	O	MET A 358	36.894	37.807	21.795	1.00	36.39	8
	ATOM	727	N	SER A 359	36.637	39.491	23.281	1.00	33.31	7
	ATOM	728	CA	SER A 359	37.860	39.226	24.019	1.00	34.39	6
	ATOM	729	CB	SER A 359	37.869	40.067	25.295	1.00	30.84	6
	ATOM	730	OG	SER A 359	39.135	40.008	25.930	1.00	47.14	8
15	ATOM	731	C	SER A 359	37.984	37.748	24.357	1.00	36.43	6
	ATOM	732	O	SER A 359	38.900	37.078	23.896	1.00	35.46	8
	ATOM	733	N	LEU A 360	37.046	37.264	25.166	1.00	36.74	7
	ATOM	734	CA	LEU A 360	37.017	35.875	25.604	1.00	35.44	6
	ATOM	735	CB	LEU A 360	35.708	35.579	26.336	1.00	34.16	6
20	ATOM	736	CG	LEU A 360	35.471	36.290	27.644	1.00	34.59	6
	ATOM	737	CD1	LEU A 360	34.225	35.765	28.312	1.00	33.53	6
	ATOM	738	CD2	LEU A 360	36.658	36.052	28.541	1.00	31.69	6
	ATOM	739	C	LEU A 360	37.203	34.862	24.500	1.00	38.72	6
	ATOM	740	O	LEU A 360	37.820	33.828	24.728	1.00	38.29	8
25	ATOM	741	N	SER A 361	36.635	35.147	23.328	1.00	40.96	7
	ATOM	742	CA	SER A 361	36.777	34.262	22.186	1.00	45.67	6
	ATOM	743	CB	SER A 361	36.518	35.045	20.904	1.00	46.45	6
	ATOM	744	OG	SER A 361	35.210	35.598	20.906	1.00	51.81	8
	ATOM	745	C	SER A 361	38.166	33.627	22.145	1.00	44.49	6
30	ATOM	746	O	SER A 361	38.347	32.538	21.625	1.00	46.67	8
	ATOM	747	N	SER A 362	39.134	34.348	22.703	1.00	41.44	7
	ATOM	748	CA	SER A 362	40.525	33.918	22.790	1.00	42.13	6
	ATOM	749	CB	SER A 362	41.408	35.131	23.066	1.00	42.61	6
	ATOM	750	OG	SER A 362	41.219	36.136	22.076	1.00	51.87	8
35	ATOM	751	C	SER A 362	40.798	32.870	23.876	1.00	38.41	6
	ATOM	752	O	SER A 362	41.553	31.938	23.641	1.00	38.01	8
	ATOM	753	N	PHE A 363	40.198	33.039	25.058	1.00	34.55	7
	ATOM	754	CA	PHE A 363	40.417	32.126	26.174	1.00	32.96	6
	ATOM	755	CB	PHE A 363	39.832	32.718	27.447	1.00	31.99	6
40	ATOM	756	CG	PHE A 363	40.448	34.036	27.840	1.00	29.97	6
	ATOM	757	CD1	PHE A 363	40.102	34.650	29.020	1.00	30.61	6
	ATOM	758	CD2	PHE A 363	41.379	34.646	27.014	1.00	32.02	6
	ATOM	759	CE1	PHE A 363	40.685	35.856	29.391	1.00	33.67	6
	ATOM	760	CE2	PHE A 363	41.959	35.843	27.377	1.00	30.91	6
45	ATOM	761	CZ	PHE A 363	41.615	36.456	28.558	1.00	29.33	6
	ATOM	762	C	PHE A 363	39.883	30.716	25.967	1.00	30.52	6
	ATOM	763	O	PHE A 363	40.436	29.766	26.526	1.00	32.19	8
	ATOM	764	N	ASN A 364	38.817	30.570	25.175	1.00	33.51	7
	ATOM	765	CA	ASN A 364	38.239	29.264	24.918	1.00	38.03	6
50	ATOM	766	CB	ASN A 364	39.240	28.404	24.139	1.00	42.32	6
	ATOM	767	CG	ASN A 364	39.696	29.065	22.861	1.00	53.11	6
	ATOM	768	OD1	ASN A 364	38.874	29.330	21.954	1.00	59.51	8
	ATOM	769	ND2	ASN A 364	40.986	29.330	22.772	1.00	55.95	7
	ATOM	770	C	ASN A 364	37.916	28.572	26.235	1.00	31.89	6
55	ATOM	771	O	ASN A 364	38.324	27.428	26.457	1.00	30.28	8
	ATOM	772	N	LEU A 365	37.176	29.271	27.094	1.00	27.62	7
	ATOM	773	CA	LEU A 365	36.806	28.743	28.406	1.00	29.36	6
	ATOM	774	CB	LEU A 365	36.195	29.866	29.237	1.00	27.54	6



5	ATOM	775	CG	LEU	A	365	36.990	31.150	29.185	1.00	38.91	6
	ATOM	776	CD1	LEU	A	365	36.316	32.216	30.036	1.00	34.47	6
	ATOM	777	CD2	LEU	A	365	38.406	30.883	29.663	1.00	34.24	6
	ATOM	778	C	LEU	A	365	35.830	27.590	28.262	1.00	26.23	6
	ATOM	779	O	LEU	A	365	34.890	27.649	27.472	1.00	27.06	8
10	ATOM	780	N	ASP	A	366	36.083	26.528	29.021	1.00	25.23	7
	ATOM	781	CA	ASP	A	366	35.213	25.358	28.988	1.00	26.07	6
	ATOM	782	CB	ASP	A	366	36.027	24.049	29.033	1.00	29.68	6
	ATOM	783	CG	ASP	A	366	36.799	23.874	30.303	1.00	35.74	6
	ATOM	784	OD1	ASP	A	366	36.285	24.177	31.402	1.00	36.78	8
15	ATOM	785	OD2	ASP	A	366	37.959	23.386	30.240	1.00	41.23	8
	ATOM	786	C	ASP	A	366	34.278	25.434	30.181	1.00	27.70	6
	ATOM	787	O	ASP	A	366	34.587	26.097	31.173	1.00	31.94	8
	ATOM	788	N	ASP	A	367	33.141	24.743	30.066	1.00	29.18	7
	ATOM	789	CA	ASP	A	367	32.120	24.679	31.120	1.00	32.72	6
20	ATOM	790	CB	ASP	A	367	31.472	23.284	31.147	1.00	38.04	6
	ATOM	791	CG	ASP	A	367	30.806	22.924	29.854	1.00	42.43	6
	ATOM	792	OD1	ASP	A	367	29.877	23.650	29.409	1.00	35.95	8
	ATOM	793	OD2	ASP	A	367	31.186	21.884	29.250	1.00	51.42	8
	ATOM	794	C	ASP	A	367	32.754	24.969	32.482	1.00	33.71	6
25	ATOM	795	O	ASP	A	367	32.484	26.000	33.098	1.00	38.30	8
	ATOM	796	N	THR	A	368	33.602	24.032	32.919	1.00	31.06	7
	ATOM	797	CA	THR	A	368	34.329	24.124	34.181	1.00	26.28	6
	ATOM	798	CB	THR	A	368	35.559	23.222	34.141	1.00	27.30	6
	ATOM	799	OG1	THR	A	368	35.161	21.871	33.885	1.00	33.42	8
30	ATOM	800	CG2	THR	A	368	36.323	23.303	35.454	1.00	25.16	6
	ATOM	801	C	THR	A	368	34.764	25.557	34.479	1.00	21.13	6
	ATOM	802	O	THR	A	368	34.408	26.153	35.503	1.00	23.17	8
	ATOM	803	N	GLU	A	369	35.545	26.092	33.551	1.00	21.32	7
	ATOM	804	CA	GLU	A	369	36.065	27.435	33.661	1.00	28.00	6
35	ATOM	805	CB	GLU	A	369	36.960	27.707	32.453	1.00	32.79	6
	ATOM	806	CG	GLU	A	369	38.089	26.663	32.346	1.00	36.29	6
	ATOM	807	CD	GLU	A	369	38.906	26.747	31.110	1.00	41.03	6
	ATOM	808	OE1	GLU	A	369	38.337	26.744	29.994	1.00	42.05	8
	ATOM	809	OE2	GLU	A	369	40.158	26.795	31.218	1.00	42.03	8
40	ATOM	810	C	GLU	A	369	34.953	28.471	33.821	1.00	25.57	6
	ATOM	811	O	GLU	A	369	34.987	29.256	34.760	1.00	20.56	8
	ATOM	812	N	VAL	A	370	33.967	28.463	32.921	1.00	25.39	7
	ATOM	813	CA	VAL	A	370	32.849	29.396	33.029	1.00	25.99	6
	ATOM	814	CB	VAL	A	370	31.763	29.131	31.987	1.00	26.15	6
45	ATOM	815	CG1	VAL	A	370	30.609	30.093	32.183	1.00	27.65	6
	ATOM	816	CG2	VAL	A	370	32.306	29.251	30.592	1.00	17.70	6
	ATOM	817	C	VAL	A	370	32.245	29.209	34.412	1.00	26.49	6
	ATOM	818	O	VAL	A	370	32.012	30.170	35.147	1.00	28.16	8
	ATOM	819	N	ALA	A	371	31.988	27.947	34.739	1.00	21.01	7
50	ATOM	820	CA	ALA	A	371	31.393	27.554	36.011	1.00	19.57	6
	ATOM	821	CB	ALA	A	371	31.441	26.039	36.145	1.00	18.62	6
	ATOM	822	C	ALA	A	371	32.116	28.211	37.177	1.00	23.48	6
	ATOM	823	O	ALA	A	371	31.531	28.989	37.931	1.00	32.67	8
	ATOM	824	N	LEU	A	372	33.401	27.893	37.305	1.00	22.89	7
55	ATOM	825	CA	LEU	A	372	34.217	28.447	38.369	1.00	23.28	6
	ATOM	826	CB	LEU	A	372	35.675	27.996	38.178	1.00	27.76	6
	ATOM	827	CG	LEU	A	372	35.943	26.524	38.415	1.00	21.18	6
	ATOM	828	CD1	LEU	A	372	37.356	26.171	38.049	1.00	27.64	6

5	ATOM	829	CD2	LEU	A	372	35.675	26.204	39.880	1.00	20.90	6
	ATOM	830	C	LEU	A	372	34.098	29.966	38.396	1.00	21.34	6
	ATOM	831	O	LEU	A	372	33.828	30.572	39.439	1.00	23.16	8
	ATOM	832	N	LEU	A	373	34.288	30.561	37.223	1.00	24.42	7
	ATOM	833	CA	LEU	A	373	34.214	32.007	37.074	1.00	23.78	6
10	ATOM	834	CB	LEU	A	373	34.296	32.360	35.575	1.00	22.18	6
	ATOM	835	CG	LEU	A	373	34.784	33.726	35.165	1.00	31.52	6
	ATOM	836	CD1	LEU	A	373	36.000	34.084	35.962	1.00	31.93	6
	ATOM	837	CD2	LEU	A	373	35.103	33.720	33.693	1.00	30.24	6
	ATOM	838	C	LEU	A	373	32.904	32.480	37.720	1.00	25.69	6
15	ATOM	839	O	LEU	A	373	32.895	33.410	38.532	1.00	30.13	8
	ATOM	840	N	GLN	A	374	31.814	31.800	37.368	1.00	26.24	7
	ATOM	841	CA	GLN	A	374	30.487	32.104	37.896	1.00	21.60	6
	ATOM	842	CB	GLN	A	374	29.454	31.121	37.335	1.00	24.57	6
	ATOM	843	CG	GLN	A	374	29.310	31.145	35.821	1.00	21.02	6
20	ATOM	844	CD	GLN	A	374	28.224	30.201	35.331	1.00	22.86	6
	ATOM	845	OE1	GLN	A	374	28.037	30.042	34.123	1.00	24.07	8
	ATOM	846	NE2	GLN	A	374	27.515	29.590	36.249	1.00	25.59	7
	ATOM	847	C	GLN	A	374	30.421	32.039	39.422	1.00	20.66	6
	ATOM	848	O	GLN	A	374	29.717	32.832	40.048	1.00	24.47	8
25	ATOM	849	N	ALA	A	375	31.136	31.074	40.004	1.00	16.26	7
	ATOM	850	CA	ALA	A	375	31.155	30.889	41.445	1.00	17.16	6
	ATOM	851	CB	ALA	A	375	31.805	29.568	41.780	1.00	19.53	6
	ATOM	852	C	ALA	A	375	31.907	32.025	42.108	1.00	25.13	6
	ATOM	853	O	ALA	A	375	31.397	32.646	43.034	1.00	23.81	8
30	ATOM	854	N	VAL	A	376	33.122	32.277	41.611	1.00	24.57	7
	ATOM	855	CA	VAL	A	376	33.959	33.354	42.118	1.00	25.80	6
	ATOM	856	CB	VAL	A	376	35.101	33.658	41.164	1.00	26.48	6
	ATOM	857	CG1	VAL	A	376	35.926	34.812	41.697	1.00	23.20	6
	ATOM	858	CG2	VAL	A	376	35.959	32.429	40.952	1.00	19.08	6
35	ATOM	859	C	VAL	A	376	33.107	34.599	42.312	1.00	25.69	6
	ATOM	860	O	VAL	A	376	33.297	35.364	43.251	1.00	27.87	8
	ATOM	861	N	LEU	A	377	32.159	34.781	41.399	1.00	23.09	7
	ATOM	862	CA	LEU	A	377	31.242	35.915	41.423	1.00	22.86	6
	ATOM	863	CB	LEU	A	377	30.540	36.031	40.061	1.00	18.50	6
40	ATOM	864	CG	LEU	A	377	31.424	36.368	38.885	1.00	22.65	6
	ATOM	865	CD1	LEU	A	377	30.689	36.227	37.601	1.00	16.70	6
	ATOM	866	CD2	LEU	A	377	31.916	37.776	39.051	1.00	19.58	6
	ATOM	867	C	LEU	A	377	30.228	35.719	42.543	1.00	26.14	6
	ATOM	868	O	LEU	A	377	30.131	36.532	43.452	1.00	20.62	8
45	ATOM	869	N	LEU	A	378	29.483	34.614	42.468	1.00	28.99	7
	ATOM	870	CA	LEU	A	378	28.469	34.303	43.475	1.00	28.87	6
	ATOM	871	CB	LEU	A	378	28.053	32.826	43.397	1.00	26.89	6
	ATOM	872	CG	LEU	A	378	27.110	32.344	44.472	1.00	28.83	6
	ATOM	873	CD1	LEU	A	378	25.915	33.252	44.525	1.00	27.97	6
50	ATOM	874	CD2	LEU	A	378	26.693	30.928	44.205	1.00	27.69	6
	ATOM	875	C	LEU	A	378	28.992	34.617	44.853	1.00	31.09	6
	ATOM	876	O	LEU	A	378	28.399	35.421	45.573	1.00	31.77	8
	ATOM	877	N	MET	A	379	30.118	33.991	45.189	1.00	31.44	7
	ATOM	878	CA	MET	A	379	30.736	34.141	46.494	1.00	32.62	6
55	ATOM	879	CB	MET	A	379	31.690	32.960	46.744	1.00	31.45	6
	ATOM	880	CG	MET	A	379	30.984	31.595	46.792	1.00	38.75	6
	ATOM	881	SD	MET	A	379	29.741	31.626	48.107	1.00	41.27	16
	ATOM	882	CE	MET	A	379	28.896	30.036	47.851	1.00	35.68	6

5	ATOM	883	C	MET A 379	31.485	35.415	46.727	1.00	53.72	6
	ATOM	884	O	MET A 379	32.567	35.450	47.305	1.00	36.29	8
	ATOM	885	N	SER A 380	30.889	36.555	46.315	1.00	34.49	7
	ATOM	886	CA	SER A 380	31.498	37.853	46.550	1.00	33.97	6
	ATOM	887	CB	SER A 380	30.921	38.890	45.576	1.00	31.24	6
10	ATOM	888	OG	SER A 380	31.205	38.543	44.230	1.00	39.42	8
	ATOM	889	C	SER A 380	31.179	38.239	47.992	1.00	39.69	6
	ATOM	890	O	SER A 380	30.029	38.446	48.357	1.00	44.64	8
	ATOM	891	N	SER A 381	32.214	38.313	48.812	1.00	41.04	7
	ATOM	892	CA	SER A 381	32.060	38.640	50.216	1.00	44.91	6
15	ATOM	893	CB	SER A 381	33.324	38.234	50.951	1.00	44.50	6
	ATOM	894	OG	SER A 381	34.431	39.002	50.510	1.00	45.42	8
	ATOM	895	C	SER A 381	31.795	40.106	50.499	1.00	44.59	6
	ATOM	896	O	SER A 381	31.476	40.470	51.618	1.00	49.32	8
	ATOM	897	N	ASP A 382	31.939	40.942	49.486	1.00	43.75	7
20	ATOM	898	CA	ASP A 382	31.744	42.362	49.641	1.00	43.93	6
	ATOM	899	CB	ASP A 382	32.673	43.111	48.677	1.00	48.39	6
	ATOM	900	CG	ASP A 382	32.572	42.624	47.263	1.00	53.23	6
	ATOM	901	OD1	ASP A 382	32.705	41.400	47.034	1.00	56.97	8
	ATOM	902	OD2	ASP A 382	32.358	43.454	46.333	1.00	58.91	8
25	ATOM	903	C	ASP A 382	30.314	42.885	49.507	1.00	41.09	6
	ATOM	904	O	ASP A 382	30.048	44.036	49.845	1.00	40.93	8
	ATOM	905	N	ARG A 383	29.397	42.049	49.034	1.00	42.63	7
	ATOM	906	CA	ARG A 383	28.036	42.485	48.876	1.00	43.32	6
	ATOM	907	CB	ARG A 383	27.138	41.332	48.443	1.00	42.31	6
30	ATOM	908	CG	ARG A 383	27.651	40.399	47.352	1.00	40.83	6
	ATOM	909	CD	ARG A 383	27.586	40.954	45.925	1.00	38.09	6
	ATOM	910	NE	ARG A 383	27.768	39.878	44.975	1.00	37.33	7
	ATOM	911	CZ	ARG A 383	28.037	40.058	43.693	1.00	38.35	6
	ATOM	912	NH1	ARG A 383	28.142	41.292	43.198	1.00	33.70	7
35	ATOM	913	NH2	ARG A 383	28.194	38.992	42.918	1.00	35.46	7
	ATOM	914	C	ARG A 383	27.523	42.989	50.216	1.00	44.96	6
	ATOM	915	O	ARG A 383	27.744	42.344	51.260	1.00	45.60	8
	ATOM	916	N	PRO A 384	26.852	44.144	50.223	1.00	45.33	7
	ATOM	917	CD	PRO A 384	26.625	44.964	49.027	1.00	46.85	6
40	ATOM	918	CA	PRO A 384	26.298	44.738	51.446	1.00	47.37	6
	ATOM	919	CB	PRO A 384	25.841	46.130	51.012	1.00	46.90	6
	ATOM	920	CG	PRO A 384	26.075	46.229	49.567	1.00	46.41	6
	ATOM	921	C	PRO A 384	25.158	43.919	52.049	1.00	48.29	6
	ATOM	922	O	PRO A 384	24.404	43.264	51.329	1.00	48.34	8
45	ATOM	923	N	GLY A 385	25.039	43.983	53.383	1.00	49.88	7
	ATOM	924	CA	GLY A 385	23.991	43.270	54.113	1.00	50.35	6
	ATOM	925	C	GLY A 385	24.347	41.852	54.495	1.00	50.70	6
	ATOM	926	O	GLY A 385	23.614	41.204	55.244	1.00	53.48	8
	ATOM	927	N	LEU A 386	25.466	41.371	53.955	1.00	49.04	7
50	ATOM	928	CA	LEU A 386	25.901	40.017	54.215	1.00	50.53	6
	ATOM	929	CB	LEU A 386	27.224	39.751	53.492	1.00	45.17	6
	ATOM	930	CG	LEU A 386	27.152	39.592	51.993	1.00	48.26	6
	ATOM	931	CD1	LEU A 386	28.542	39.439	51.404	1.00	41.68	6
	ATOM	932	CD2	LEU A 386	26.302	38.374	51.682	1.00	38.40	6
55	ATOM	933	C	LEU A 386	26.045	39.776	55.691	1.00	52.13	6
	ATOM	934	O	LEU A 386	26.296	40.692	56.459	1.00	53.67	8
	ATOM	935	N	ALA A 387	25.861	38.522	56.077	1.00	53.42	7
	ATOM	936	CA	ALA A 387	25.976	38.129	57.470	1.00	56.01	6

5	ATOM	937	CB	ALA	A	387	24.802	37.234	57.554	1.00	56.47	6
	ATOM	938	C	ALA	A	387	27.289	37.385	57.659	1.00	55.52	6
	ATOM	939	O	ALA	A	387	28.275	37.940	58.134	1.00	53.75	8
	ATOM	940	N	CYS	A	388	27.273	36.120	57.253	1.00	56.03	7
	ATOM	941	CA	CYS	A	388	28.412	35.236	57.370	1.00	59.57	6
10	ATOM	942	CB	CYS	A	388	27.923	33.803	57.172	1.00	59.23	6
	ATOM	943	SG	CYS	A	388	26.397	33.431	58.009	1.00	58.64	16
	ATOM	944	C	CYS	A	388	29.482	35.581	56.328	1.00	62.18	6
	ATOM	945	O	CYS	A	388	29.720	34.821	55.400	1.00	67.88	8
	ATOM	946	N	VAL	A	389	30.110	36.747	56.495	1.00	60.78	7
15	ATOM	947	CA	VAL	A	389	31.173	37.212	55.590	1.00	57.70	6
	ATOM	948	CB	VAL	A	389	31.740	38.567	56.024	1.00	57.09	6
	ATOM	949	CG1	VAL	A	389	32.795	39.037	55.041	1.00	59.03	6
	ATOM	950	CG2	VAL	A	389	30.640	39.598	56.171	1.00	53.98	6
	ATOM	951	C	VAL	A	389	32.297	36.182	55.550	1.00	57.77	6
20	ATOM	952	O	VAL	A	389	32.358	35.336	54.662	1.00	60.94	8
	ATOM	953	N	ALA	A	390	33.182	36.292	56.528	1.00	52.68	7
	ATOM	954	CA	ALA	A	390	34.347	35.431	56.684	1.00	48.41	6
	ATOM	955	CB	ALA	A	390	34.703	35.321	58.185	1.00	45.19	6
	ATOM	956	C	ALA	A	390	34.224	34.040	56.082	1.00	47.63	6
25	ATOM	957	O	ALA	A	390	35.107	33.597	55.348	1.00	51.95	8
	ATOM	958	N	ARG	A	391	33.117	33.366	56.391	1.00	47.11	7
	ATOM	959	CA	ARG	A	391	32.879	32.018	55.885	1.00	51.64	6
	ATOM	960	CB	ARG	A	391	31.520	31.498	56.383	1.00	54.22	6
	ATOM	961	CG	ARG	A	391	31.267	30.012	56.059	1.00	64.20	6
30	ATOM	962	CD	ARG	A	391	29.930	29.489	56.602	1.00	73.80	6
	ATOM	963	NE	ARG	A	391	29.787	28.044	56.454	1.00	79.76	7
	ATOM	964	CZ	ARG	A	391	30.573	27.140	57.043	1.00	84.27	6
	ATOM	965	NH1	ARG	A	391	31.598	27.535	57.806	1.00	85.28	7
	ATOM	966	NH2	ARG	A	391	30.340	25.840	56.849	1.00	86.84	7
35	ATOM	967	C	ARG	A	391	32.922	31.986	54.358	1.00	48.18	6
	ATOM	968	O	ARG	A	391	33.494	31.080	53.756	1.00	49.57	8
	ATOM	969	N	ILE	A	392	32.281	32.993	53.762	1.00	45.01	7
	ATOM	970	CA	ILE	A	392	32.196	33.148	52.319	1.00	48.77	6
	ATOM	971	CB	ILE	A	392	31.224	34.297	51.963	1.00	46.45	6
40	ATOM	972	CG2	ILE	A	392	31.241	34.582	50.479	1.00	42.35	6
	ATOM	973	CG1	ILE	A	392	29.791	33.953	52.402	1.00	49.69	6
	ATOM	974	CD1	ILE	A	392	28.792	35.039	52.113	1.00	51.09	6
	ATOM	975	C	ILE	A	392	33.554	33.356	51.641	1.00	50.90	6
	ATOM	976	O	ILE	A	392	33.914	32.605	50.732	1.00	52.21	8
45	ATOM	977	N	GLU	A	393	34.298	34.374	52.071	1.00	50.43	7
	ATOM	978	CA	GLU	A	393	35.592	34.684	51.471	1.00	50.30	6
	ATOM	979	CB	GLU	A	393	36.437	35.561	52.387	1.00	53.97	6
	ATOM	980	CG	GLU	A	393	36.558	36.966	51.844	1.00	62.18	6
	ATOM	981	CD	GLU	A	393	37.546	37.777	52.564	1.00	67.69	6
50	ATOM	982	OE1	GLU	A	393	38.149	38.741	52.119	1.00	66.42	8
	ATOM	983	OE2	GLU	A	393	37.856	37.640	53.729	1.00	70.64	8
	ATOM	984	C	GLU	A	393	36.341	33.429	51.230	1.00	49.31	6
	ATOM	985	O	GLU	A	393	36.755	33.089	50.125	1.00	49.53	8
	ATOM	986	N	LYS	A	394	36.552	32.730	52.303	1.00	46.07	7
55	ATOM	987	CA	LYS	A	394	37.265	31.543	52.078	1.00	45.76	6
	ATOM	988	CB	LYS	A	394	37.396	30.800	53.373	1.00	43.85	6
	ATOM	989	CG	LYS	A	394	38.207	31.617	54.394	1.00	40.00	6
	ATOM	990	CD	LYS	A	394	39.372	32.374	53.705	1.00	40.00	6

5	ATOM	991	CE	LYS	A	394	40.136	<del>38.265</del>	<del>54.689</del>	<del>1.00</del>	40.00	6
	ATOM	992	NZ	LYS	A	394	41.516	33.602	54.162	1.00	40.00	7
	ATOM	993	C	LYS	A	394	36.568	30.778	50.966	1.00	46.69	6
	ATOM	994	O	LYS	A	394	37.215	30.427	49.988	1.00	49.13	8
	ATOM	995	N	TYR	A	395	35.269	30.514	51.095	1.00	46.57	7
10	ATOM	996	CA	TYR	A	395	34.553	29.823	50.022	1.00	43.33	6
	ATOM	997	CB	TYR	A	395	33.059	30.123	50.076	1.00	48.44	6
	ATOM	998	CG	TYR	A	395	32.275	29.236	50.994	1.00	53.83	6
	ATOM	999	CD1	TYR	A	395	31.010	29.598	51.415	1.00	56.43	6
	ATOM	1000	CE1	TYR	A	395	30.266	28.769	52.252	1.00	59.73	6
15	ATOM	1001	CD2	TYR	A	395	32.790	28.033	51.428	1.00	56.47	6
	ATOM	1002	CE2	TYR	A	395	32.054	27.198	52.265	1.00	62.60	6
	ATOM	1003	CZ	TYR	A	395	30.787	27.565	52.687	1.00	63.18	6
	ATOM	1004	OH	TYR	A	395	30.059	26.753	53.528	1.00	64.46	8
	ATOM	1005	C	TYR	A	395	35.120	30.356	48.716	1.00	37.30	6
20	ATOM	1006	O	TYR	A	395	35.643	29.601	47.908	1.00	34.10	8
	ATOM	1007	N	GLN	A	396	35.029	31.670	48.522	1.00	31.92	7
	ATOM	1008	CA	GLN	A	396	35.563	32.273	47.305	1.00	34.81	6
	ATOM	1009	CB	GLN	A	396	35.403	33.801	47.329	1.00	32.64	6
	ATOM	1010	CG	GLN	A	396	36.088	34.485	46.162	1.00	29.57	6
25	ATOM	1011	CD	GLN	A	396	35.616	35.891	45.927	1.00	29.46	6
	ATOM	1012	OE1	GLN	A	396	35.599	36.726	46.862	1.00	34.65	8
	ATOM	1013	NE2	GLN	A	396	35.245	36.173	44.689	1.00	27.21	7
	ATOM	1014	C	GLN	A	396	37.035	31.909	47.167	1.00	37.13	6
	ATOM	1015	O	GLN	A	396	37.511	31.590	46.080	1.00	37.36	8
30	ATOM	1016	N	ASP	A	397	37.751	31.970	48.285	1.00	38.61	7
	ATOM	1017	CA	ASP	A	397	39.164	31.642	48.298	1.00	40.37	6
	ATOM	1018	CB	ASP	A	397	39.757	31.869	49.704	1.00	40.51	6
	ATOM	1019	CG	ASP	A	397	39.813	33.319	50.095	1.00	43.77	6
	ATOM	1020	OD1	ASP	A	397	40.397	34.123	49.334	1.00	46.50	8
35	ATOM	1021	OD2	ASP	A	397	39.299	33.702	51.184	1.00	51.34	8
	ATOM	1022	C	ASP	A	397	39.302	30.176	47.898	1.00	38.62	6
	ATOM	1023	O	ASP	A	397	40.230	29.809	47.199	1.00	39.20	8
	ATOM	1024	N	SER	A	398	38.350	29.359	48.344	1.00	37.84	7
	ATOM	1025	CA	SER	A	398	38.348	27.929	48.063	1.00	37.80	6
40	ATOM	1026	CB	SER	A	398	37.240	27.240	48.878	1.00	34.28	6
	ATOM	1027	OG	SER	A	398	37.297	25.826	48.755	1.00	46.60	8
	ATOM	1028	C	SER	A	398	38.164	27.639	46.581	1.00	38.41	6
	ATOM	1029	O	SER	A	398	38.677	26.642	46.075	1.00	39.98	8
	ATOM	1030	N	PHE	A	399	37.419	28.507	45.893	1.00	34.82	7
45	ATOM	1031	CA	PHE	A	399	37.181	28.325	44.462	1.00	35.96	6
	ATOM	1032	CB	PHE	A	399	35.873	28.983	44.015	1.00	35.75	6
	ATOM	1033	CG	PHE	A	399	34.632	28.216	44.403	1.00	39.30	6
	ATOM	1034	CD1	PHE	A	399	34.107	28.294	45.677	1.00	39.86	6
	ATOM	1035	CD2	PHE	A	399	34.018	27.393	43.488	1.00	36.81	6
50	ATOM	1036	CE1	PHE	A	399	32.961	27.557	46.013	1.00	41.25	6
	ATOM	1037	CE2	PHE	A	399	32.880	26.661	43.825	1.00	43.61	6
	ATOM	1038	CZ	PHE	A	399	32.354	26.740	45.087	1.00	40.34	6
	ATOM	1039	C	PHE	A	399	38.328	28.890	43.630	1.00	33.48	6
	ATOM	1040	O	PHE	A	399	38.867	28.200	42.756	1.00	26.86	8
55	ATOM	1041	N	LEU	A	400	38.680	30.156	43.877	1.00	31.47	7
	ATOM	1042	CA	LEU	A	400	39.754	30.796	43.132	1.00	37.41	6
	ATOM	1043	CB	LEU	A	400	40.179	32.100	43.814	1.00	34.24	6
	ATOM	1044	CG	LEU	A	400	39.239	33.265	43.628	1.00	35.10	6

5	ATOM	1045	CD1	LEU	A	400	39.803	<del>34.531</del>	44.256	1.00	26.60	6
	ATOM	1046	CD2	LEU	A	400	39.065	33.479	42.137	1.00	29.44	6
	ATOM	1047	C	LEU	A	400	40.941	29.872	42.947	1.00	38.84	6
	ATOM	1048	O	LEU	A	400	41.367	29.632	41.821	1.00	40.38	8
	ATOM	1049	N	LEU	A	401	41.464	29.350	44.055	1.00	42.79	7
10	ATOM	1050	CA	LEU	A	401	42.605	28.449	43.988	1.00	43.48	6
	ATOM	1051	CB	LEU	A	401	42.900	27.821	45.355	1.00	44.73	6
	ATOM	1052	CG	LEU	A	401	44.105	26.899	45.354	1.00	51.39	6
	ATOM	1053	CD1	LEU	A	401	45.374	27.749	45.143	1.00	50.11	6
	ATOM	1054	CD2	LEU	A	401	44.205	26.122	46.662	1.00	49.30	6
15	ATOM	1055	C	LEU	A	401	42.324	27.340	42.981	1.00	41.62	6
	ATOM	1056	O	LEU	A	401	43.052	27.180	42.004	1.00	45.14	8
	ATOM	1057	N	ALA	A	402	41.269	26.574	43.245	1.00	37.92	7
	ATOM	1058	CA	ALA	A	402	40.873	25.469	42.386	1.00	29.90	6
	ATOM	1059	CB	ALA	A	402	39.522	24.928	42.834	1.00	30.70	6
20	ATOM	1060	C	ALA	A	402	40.798	25.909	40.929	1.00	28.88	6
	ATOM	1061	O	ALA	A	402	41.277	25.203	40.034	1.00	32.14	8
	ATOM	1062	N	PHE	A	403	40.200	27.086	40.707	1.00	31.07	7
	ATOM	1063	CA	PHE	A	403	40.052	27.642	39.363	1.00	29.90	6
	ATOM	1064	CB	PHE	A	403	39.379	29.019	39.438	1.00	27.03	6
25	ATOM	1065	CG	PHE	A	403	38.943	29.574	38.100	1.00	26.97	6
	ATOM	1066	CD1	PHE	A	403	38.228	30.758	38.033	1.00	25.55	6
	ATOM	1067	CD2	PHE	A	403	39.224	28.905	36.925	1.00	19.75	6
	ATOM	1068	CE1	PHE	A	403	37.784	31.266	36.808	1.00	27.90	6
	ATOM	1069	CE2	PHE	A	403	38.780	29.416	35.694	1.00	22.56	6
30	ATOM	1070	CZ	PHE	A	403	38.063	30.596	35.640	1.00	22.24	6
	ATOM	1071	C	PHE	A	403	41.429	27.756	38.719	1.00	28.82	6
	ATOM	1072	O	PHE	A	403	41.666	27.210	37.646	1.00	26.00	8
	ATOM	1073	N	GLU	A	404	42.329	28.463	39.402	1.00	30.25	7
	ATOM	1074	CA	GLU	A	404	43.695	28.665	38.922	1.00	34.03	6
35	ATOM	1075	CB	GLU	A	404	44.513	29.416	39.983	1.00	39.45	6
	ATOM	1076	CG	GLU	A	404	45.867	29.935	39.489	1.00	47.68	6
	ATOM	1077	CD	GLU	A	404	46.734	30.507	40.571	1.00	54.02	6
	ATOM	1078	OE1	GLU	A	404	46.236	31.298	41.408	1.00	57.27	8
	ATOM	1079	OE2	GLU	A	404	47.956	30.202	40.606	1.00	63.85	8
40	ATOM	1080	C	GLU	A	404	44.352	27.322	38.634	1.00	36.01	6
	ATOM	1081	O	GLU	A	404	44.936	27.112	37.574	1.00	38.64	8
	ATOM	1082	N	HIS	A	405	44.259	26.420	39.610	1.00	29.56	7
	ATOM	1083	CA	HIS	A	405	44.840	25.093	39.468	1.00	31.69	6
	ATOM	1084	CB	HIS	A	405	44.540	24.228	40.694	1.00	33.75	6
45	ATOM	1085	CG	HIS	A	405	45.292	24.657	41.908	1.00	34.75	6
	ATOM	1086	CD2	HIS	A	405	46.198	25.640	42.130	1.00	34.58	6
	ATOM	1087	ND1	HIS	A	405	45.161	23.984	43.130	1.00	32.43	7
	ATOM	1088	CE1	HIS	A	405	45.975	24.568	44.018	1.00	36.15	6
	ATOM	1089	NE2	HIS	A	405	46.601	25.561	43.430	1.00	39.84	7
50	ATOM	1090	C	HIS	A	405	44.274	24.445	38.225	1.00	34.21	6
	ATOM	1091	O	HIS	A	405	45.029	23.949	37.386	1.00	37.06	8
	ATOM	1092	N	TYR	A	406	42.947	24.453	38.100	1.00	30.83	7
	ATOM	1093	CA	TYR	A	406	42.313	23.859	36.930	1.00	28.85	6
	ATOM	1094	CB	TYR	A	406	40.805	24.080	36.934	1.00	31.48	6
55	ATOM	1095	CG	TYR	A	406	40.139	23.494	35.709	1.00	23.49	6
	ATOM	1096	CD1	TYR	A	406	40.073	22.123	35.532	1.00	19.42	6
	ATOM	1097	CE1	TYR	A	406	39.517	21.577	34.382	1.00	23.80	6
	ATOM	1098	CD2	TYR	A	406	39.646	24.313	34.704	1.00	21.81	6

5	ATOM	1099	CE2	TYR	A	406	39.090	23.361	33.351	1.00	21.64	6
	ATOM	1100	CZ	TYR	A	406	39.029	22.395	33.380	1.00	21.56	6
	ATOM	1101	OH	TYR	A	406	38.489	21.850	32.236	1.00	24.96	8
	ATOM	1102	C	TYR	A	406	42.882	24.504	35.672	1.00	24.24	6
	ATOM	1103	O	TYR	A	406	42.958	23.872	34.621	1.00	27.08	8
10	ATOM	1104	N	ILE	A	407	43.253	25.784	35.807	1.00	25.76	7
	ATOM	1105	CA	ILE	A	407	43.824	26.548	34.705	1.00	33.75	6
	ATOM	1106	CB	ILE	A	407	43.986	28.033	35.070	1.00	34.23	6
	ATOM	1107	CG2	ILE	A	407	44.967	28.712	34.139	1.00	32.46	6
	ATOM	1108	CG1	ILE	A	407	42.615	28.728	35.042	1.00	43.30	6
15	ATOM	1109	CD1	ILE	A	407	41.896	28.602	33.694	1.00	40.40	6
	ATOM	1110	C	ILE	A	407	45.143	25.973	34.256	1.00	39.03	6
	ATOM	1111	O	ILE	A	407	45.383	25.771	33.063	1.00	35.18	8
	ATOM	1112	N	ASN	A	408	46.003	25.721	35.227	1.00	37.25	7
	ATOM	1113	CA	ASN	A	408	47.307	25.194	34.926	1.00	37.01	6
20	ATOM	1114	CB	ASN	A	408	48.107	25.017	36.213	1.00	32.27	6
	ATOM	1115	CG	ASN	A	408	48.346	26.362	36.936	1.00	33.56	6
	ATOM	1116	OD1	ASN	A	408	48.827	27.335	36.320	1.00	31.99	8
	ATOM	1117	ND2	ASN	A	408	48.038	26.403	38.231	1.00	31.23	7
	ATOM	1118	C	ASN	A	408	47.205	23.892	34.136	1.00	38.14	6
25	ATOM	1119	O	ASN	A	408	47.900	23.734	33.124	1.00	42.16	8
	ATOM	1120	N	TYR	A	409	46.334	22.981	34.568	1.00	35.62	7
	ATOM	1121	CA	TYR	A	409	46.159	21.710	33.866	1.00	35.91	6
	ATOM	1122	CB	TYR	A	409	45.051	20.859	34.507	1.00	34.41	6
	ATOM	1123	CG	TYR	A	409	44.624	19.687	33.619	1.00	38.73	6
30	ATOM	1124	CD1	TYR	A	409	45.563	18.765	33.155	1.00	41.34	6
	ATOM	1125	CE1	TYR	A	409	45.186	17.709	32.321	1.00	47.16	6
	ATOM	1126	CD2	TYR	A	409	43.292	19.515	33.232	1.00	46.20	6
	ATOM	1127	CE2	TYR	A	409	42.913	18.455	32.397	1.00	50.74	6
	ATOM	1128	CZ	TYR	A	409	43.863	17.551	31.946	1.00	50.88	6
35	ATOM	1129	OH	TYR	A	409	43.498	16.514	31.130	1.00	53.14	8
	ATOM	1130	C	TYR	A	409	45.760	21.966	32.424	1.00	38.16	6
	ATOM	1131	O	TYR	A	409	46.202	21.281	31.502	1.00	41.83	8
	ATOM	1132	N	ARG	A	410	44.872	22.943	32.272	1.00	42.25	7
	ATOM	1133	CA	ARG	A	410	44.345	23.332	30.984	1.00	42.83	6
40	ATOM	1134	CB	ARG	A	410	43.311	24.427	31.195	1.00	36.83	6
	ATOM	1135	CG	ARG	A	410	41.994	23.979	31.795	1.00	34.32	6
	ATOM	1136	CD	ARG	A	410	41.073	23.504	30.675	1.00	36.62	6
	ATOM	1137	NE	ARG	A	410	40.888	24.550	29.685	1.00	38.64	7
	ATOM	1138	CZ	ARG	A	410	40.177	24.397	28.576	1.00	35.73	6
45	ATOM	1139	NH1	ARG	A	410	39.572	23.230	28.348	1.00	33.17	7
	ATOM	1140	NH2	ARG	A	410	40.077	25.407	27.708	1.00	32.70	7
	ATOM	1141	C	ARG	A	410	45.442	23.850	30.083	1.00	46.67	6
	ATOM	1142	O	ARG	A	410	45.467	23.591	28.882	1.00	41.78	8
	ATOM	1143	N	LYS	A	411	46.360	24.577	30.710	1.00	52.99	7
50	ATOM	1144	CA	LYS	A	411	47.467	25.194	30.017	1.00	58.32	6
	ATOM	1145	CB	LYS	A	411	48.645	24.216	29.876	1.00	64.99	6
	ATOM	1146	CG	LYS	A	411	48.349	22.835	29.367	1.00	70.48	6
	ATOM	1147	CD	LYS	A	411	49.608	21.974	29.494	1.00	77.18	6
	ATOM	1148	CE	LYS	A	411	49.461	20.621	28.795	1.00	84.30	6
55	ATOM	1149	NZ	LYS	A	411	50.740	19.828	28.857	1.00	86.48	7
	ATOM	1150	C	LYS	A	411	47.032	25.756	28.686	1.00	56.66	6
	ATOM	1151	O	LYS	A	411	47.160	25.153	27.633	1.00	55.47	8
	ATOM	1152	N	HIS	A	412	46.458	26.943	28.823	1.00	54.67	7

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					45.984	27.722	27.705	1.00	48.67	6
5	ATOM	1153	CA	HIS A 412	45.124	28.884	28.201	1.00	43.14	6
	ATOM	1154	CB	HIS A 412	43.812	28.480	28.755	1.00	41.36	6
	ATOM	1155	CG	HIS A 412	43.429	28.064	29.987	1.00	35.44	6
	ATOM	1156	CD2	HIS A 412	42.651	28.440	27.966	1.00	38.19	7
	ATOM	1157	ND1	HIS A 412	41.648	28.014	28.723	1.00	34.75	6
10	ATOM	1158	CE1	HIS A 412	42.094	27.780	29.942	1.00	35.52	7
	ATOM	1159	NE2	HIS A 412	47.231	28.303	27.101	1.00	46.35	6
	ATOM	1160	C	HIS A 412	48.269	28.452	27.775	1.00	42.73	8
	ATOM	1161	O	HIS A 412	47.116	28.696	25.839	1.00	48.92	7
	ATOM	1162	N	HIS A 413	48.234	29.290	25.146	1.00	53.15	6
15	ATOM	1163	CA	HIS A 413	48.404	28.666	23.755	1.00	55.27	6
	ATOM	1164	CB	HIS A 413	49.326	29.446	22.886	1.00	58.77	6
	ATOM	1165	CG	HIS A 413	49.213	30.660	22.304	1.00	61.65	6
	ATOM	1166	CD2	HIS A 413	50.617	28.997	22.564	1.00	60.31	7
	ATOM	1167	ND1	HIS A 413	51.214	29.924	21.828	1.00	63.01	6
20	ATOM	1168	CE1	HIS A 413	50.386	30.941	21.658	1.00	62.93	7
	ATOM	1169	NE2	HIS A 413	47.932	30.768	24.998	1.00	53.19	6
	ATOM	1170	C	HIS A 413	47.639	31.301	23.934	1.00	54.93	8
	ATOM	1171	O	HIS A 413	47.964	31.413	26.139	1.00	53.77	7
	ATOM	1172	N	VAL A 414	47.735	32.811	26.146	1.00	51.06	6
25	ATOM	1173	CA	VAL A 414	46.291	33.183	26.417	1.00	51.49	6
	ATOM	1174	CB	VAL A 414	46.186	34.715	26.603	1.00	45.22	6
	ATOM	1175	CG1	VAL A 414	45.419	32.732	25.263	1.00	52.67	6
	ATOM	1176	CG2	VAL A 414	48.623	33.283	27.226	1.00	54.28	6
	ATOM	1177	C	VAL A 414	48.427	33.029	28.409	1.00	55.49	8
30	ATOM	1178	O	VAL A 414	49.706	33.863	26.733	1.00	56.28	7
	ATOM	1179	N	THR A 415	50.721	34.484	27.557	1.00	57.83	6
	ATOM	1180	CA	THR A 415	51.268	35.675	26.758	1.00	59.64	6
	ATOM	1181	CB	THR A 415	51.605	36.754	27.636	1.00	66.69	8
	ATOM	1182	OG1	THR A 415	50.197	36.158	25.745	1.00	59.42	6
35	ATOM	1183	CG2	THR A 415	50.146	35.049	28.879	1.00	56.98	6
	ATOM	1184	C	THR A 415	48.933	35.146	29.051	1.00	55.70	8
	ATOM	1185	O	THR A 415	51.068	35.330	29.795	1.00	57.44	7
	ATOM	1186	N	HIS A 416	50.808	36.011	31.047	1.00	57.34	6
	ATOM	1187	CA	HIS A 416	51.346	37.422	30.708	1.00	61.35	6
40	ATOM	1188	CB	HIS A 416	51.872	38.237	31.821	1.00	69.78	6
	ATOM	1189	CG	HIS A 416	53.114	38.297	32.390	1.00	71.42	6
	ATOM	1190	CD2	HIS A 416	51.135	39.263	32.416	1.00	72.49	7
	ATOM	1191	ND1	HIS A 416	51.914	39.884	33.290	1.00	75.50	6
	ATOM	1192	CE1	HIS A 416	53.099	39.323	33.291	1.00	73.91	7
45	ATOM	1193	NE2	HIS A 416	49.261	35.892	31.297	1.00	53.79	6
	ATOM	1194	C	HIS A 416	48.499	36.779	30.902	1.00	52.81	8
	ATOM	1195	O	HIS A 416	48.806	34.779	31.911	1.00	48.05	7
	ATOM	1196	N	PHE A 417	47.355	34.428	32.061	1.00	47.99	6
	ATOM	1197	CA	PHE A 417	47.165	32.954	31.996	1.00	46.11	6
50	ATOM	1198	CB	PHE A 417	45.835	32.590	31.399	1.00	44.27	6
	ATOM	1199	CG	PHE A 417	45.680	32.720	30.046	1.00	41.79	6
	ATOM	1200	CD1	PHE A 417	44.758	32.135	32.164	1.00	40.23	6
	ATOM	1201	CD2	PHE A 417	44.498	32.397	29.422	1.00	44.30	6
	ATOM	1202	CE1	PHE A 417	43.540	31.802	31.529	1.00	36.80	6
55	ATOM	1203	CE2	PHE A 417	43.427	31.928	30.144	1.00	40.69	6
	ATOM	1204	CZ	PHE A 417	46.427	34.836	33.196	1.00	46.69	6
	ATOM	1205	C	PHE A 417	46.147	36.004	33.331	1.00	43.35	8
	ATOM	1206	O	PHE A 417						



5	ATOM	1207	N	TRP	A	418	45.906	33.801	33.909	1.00	45.14	7
	ATOM	1208	CA	TRP	A	418	44.982	33.867	35.065	1.00	44.89	6
	ATOM	1209	CB	TRP	A	418	45.545	33.099	36.255	1.00	42.24	6
	ATOM	1210	CG	TRP	A	418	44.959	33.452	37.598	1.00	47.11	6
	ATOM	1211	CD2	TRP	A	418	43.724	32.924	38.149	1.00	46.98	6
10	ATOM	1212	CE2	TRP	A	418	43.534	33.565	39.413	1.00	48.94	6
	ATOM	1213	CE3	TRP	A	418	42.777	31.986	37.688	1.00	45.23	6
	ATOM	1214	CD1	TRP	A	418	45.434	34.350	38.512	1.00	46.24	6
	ATOM	1215	NE1	TRP	A	418	44.588	34.407	39.608	1.00	50.63	7
	ATOM	1216	CZ2	TRP	A	418	42.441	33.270	40.238	1.00	45.46	6
15	ATOM	1217	CZ3	TRP	A	418	41.686	31.706	38.500	1.00	44.50	6
	ATOM	1218	CH2	TRP	A	418	41.511	32.335	39.753	1.00	47.55	6
	ATOM	1219	C	TRP	A	418	44.908	35.324	35.398	1.00	43.88	6
	ATOM	1220	O	TRP	A	418	43.797	35.839	35.702	1.00	43.17	8
	ATOM	1221	N	PRO	A	419	46.084	35.976	35.461	1.00	43.55	7
20	ATOM	1222	CD	PRO	A	419	47.467	35.482	35.400	1.00	41.52	6
	ATOM	1223	CA	PRO	A	419	46.009	37.396	35.758	1.00	41.48	6
	ATOM	1224	CB	PRO	A	419	47.436	37.884	35.535	1.00	39.21	6
	ATOM	1225	CG	PRO	A	419	48.261	36.696	35.223	1.00	39.25	6
	ATOM	1226	C	PRO	A	419	44.960	38.090	34.817	1.00	36.28	6
25	ATOM	1227	O	PRO	A	419	44.208	38.978	35.237	1.00	37.08	8
	ATOM	1228	N	LYS	A	420	44.915	37.701	33.540	1.00	35.96	7
	ATOM	1229	CA	LYS	A	420	43.977	38.287	32.575	1.00	40.82	6
	ATOM	1230	CB	LYS	A	420	44.314	37.805	31.155	1.00	40.78	6
	ATOM	1231	CG	LYS	A	420	45.684	38.244	30.641	1.00	48.62	6
30	ATOM	1232	CD	LYS	A	420	45.904	37.781	29.206	1.00	55.12	6
	ATOM	1233	CE	LYS	A	420	47.248	38.261	28.673	1.00	53.26	6
	ATOM	1234	NZ	LYS	A	420	47.448	37.884	27.222	1.00	52.69	7
	ATOM	1235	C	LYS	A	420	42.580	37.832	32.948	1.00	40.29	6
	ATOM	1236	O	LYS	A	420	41.656	38.626	32.982	1.00	39.66	8
35	ATOM	1237	N	LEU	A	421	42.461	36.537	33.245	1.00	38.33	7
	ATOM	1238	CA	LEU	A	421	41.186	35.931	33.613	1.00	37.60	6
	ATOM	1239	CB	LEU	A	421	41.397	34.433	33.915	1.00	43.66	6
	ATOM	1240	CG	LEU	A	421	40.204	33.518	33.828	1.00	46.50	6
	ATOM	1241	CD1	LEU	A	421	39.643	33.624	32.426	1.00	45.15	6
40	ATOM	1242	CD2	LEU	A	421	40.595	32.094	34.131	1.00	51.31	6
	ATOM	1243	C	LEU	A	421	40.575	36.664	34.808	1.00	39.59	6
	ATOM	1244	O	LEU	A	421	39.371	36.910	34.837	1.00	40.66	8
	ATOM	1245	N	LEU	A	422	41.412	37.017	35.782	1.00	39.57	7
	ATOM	1246	CA	LEU	A	422	40.946	37.726	36.961	1.00	38.63	6
45	ATOM	1247	CB	LEU	A	422	42.085	37.890	37.971	1.00	41.79	6
	ATOM	1248	CG	LEU	A	422	42.424	36.671	38.798	1.00	42.74	6
	ATOM	1249	CD1	LEU	A	422	43.490	37.010	39.820	1.00	42.89	6
	ATOM	1250	CD2	LEU	A	422	41.168	36.216	39.523	1.00	39.27	6
	ATOM	1251	C	LEU	A	422	40.381	39.073	36.589	1.00	40.47	6
50	ATOM	1252	O	LEU	A	422	39.428	39.525	37.210	1.00	47.83	8
	ATOM	1253	N	MET	A	423	40.969	39.698	35.569	1.00	34.27	7
	ATOM	1254	CA	MET	A	423	40.511	41.001	35.117	1.00	35.25	6
	ATOM	1255	CB	MET	A	423	41.427	41.553	34.028	1.00	32.56	6
	ATOM	1256	CG	MET	A	423	42.856	41.732	34.456	1.00	40.70	6
55	ATOM	1257	SD	MET	A	423	43.707	43.101	33.619	1.00	47.65	16
	ATOM	1258	CE	MET	A	423	43.348	42.776	31.848	1.00	47.16	6
	ATOM	1259	C	MET	A	423	39.100	40.899	34.574	1.00	35.13	6
	ATOM	1260	O	MET	A	423	38.315	41.829	34.696	1.00	29.85	8

5	ATOM	1261	N	LYS A 424	38.791	39.752	33.975	1.00	31.56	7
	ATOM	1262	CA	LYS A 424	37.470	39.529	33.423	1.00	32.29	6
	ATOM	1263	CB	LYS A 424	37.446	38.205	32.658	1.00	30.56	6
	ATOM	1264	CG	LYS A 424	38.394	38.192	31.455	1.00	30.07	6
	ATOM	1265	CD	LYS A 424	38.050	39.326	30.488	1.00	33.22	6
10	ATOM	1266	CE	LYS A 424	39.032	39.433	29.322	1.00	28.75	6
	ATOM	1267	NZ	LYS A 424	40.394	39.942	29.707	1.00	31.01	7
	ATOM	1268	C	LYS A 424	36.418	39.558	34.524	1.00	29.26	6
	ATOM	1269	O	LYS A 424	35.307	39.998	34.289	1.00	30.22	8
	ATOM	1270	N	VAL A 425	36.796	39.098	35.719	1.00	23.53	7
15	ATOM	1271	CA	VAL A 425	35.897	39.107	36.866	1.00	28.91	6
	ATOM	1272	CB	VAL A 425	36.541	38.460	38.094	1.00	29.44	6
	ATOM	1273	CG1	VAL A 425	35.673	38.642	39.320	1.00	28.81	6
	ATOM	1274	CG2	VAL A 425	36.764	36.985	37.849	1.00	31.22	6
	ATOM	1275	C	VAL A 425	35.512	40.548	37.161	1.00	32.03	6
20	ATOM	1276	O	VAL A 425	34.350	40.839	37.429	1.00	31.95	8
	ATOM	1277	N	THR A 426	36.496	41.444	37.124	1.00	33.61	7
	ATOM	1278	CA	THR A 426	36.248	42.866	37.356	1.00	30.76	6
	ATOM	1279	CB	THR A 426	37.559	43.670	37.360	1.00	32.34	6
	ATOM	1280	OG1	THR A 426	38.209	43.565	38.630	1.00	33.07	8
25	ATOM	1281	CG2	THR A 426	37.302	45.131	37.015	1.00	25.40	6
	ATOM	1282	C	THR A 426	35.363	43.324	36.211	1.00	32.53	6
	ATOM	1283	O	THR A 426	34.357	44.006	36.405	1.00	35.19	8
	ATOM	1284	N	ASP A 427	35.763	42.929	35.006	1.00	28.83	7
	ATOM	1285	CA	ASP A 427	35.011	43.272	33.810	1.00	35.12	6
30	ATOM	1286	CB	ASP A 427	35.556	42.524	32.578	1.00	39.14	6
	ATOM	1287	CG	ASP A 427	36.837	43.103	32.057	1.00	45.80	6
	ATOM	1288	OD1	ASP A 427	36.982	44.346	32.024	1.00	41.97	8
	ATOM	1289	OD2	ASP A 427	37.735	42.333	31.616	1.00	50.06	8
	ATOM	1290	C	ASP A 427	33.537	42.925	34.028	1.00	33.94	6
35	ATOM	1291	O	ASP A 427	32.659	43.712	33.702	1.00	38.02	8
	ATOM	1292	N	LEU A 428	33.283	41.745	34.584	1.00	27.15	7
	ATOM	1293	CA	LEU A 428	31.925	41.293	34.850	1.00	29.99	6
	ATOM	1294	CB	LEU A 428	31.924	39.786	35.133	1.00	22.49	6
	ATOM	1295	CG	LEU A 428	32.104	38.873	33.939	1.00	25.54	6
40	ATOM	1296	CD1	LEU A 428	32.202	37.421	34.353	1.00	20.60	6
	ATOM	1297	CD2	LEU A 428	30.920	39.083	33.029	1.00	17.24	6
	ATOM	1298	C	LEU A 428	31.276	42.057	35.991	1.00	28.94	6
	ATOM	1299	O	LEU A 428	30.082	42.306	35.939	1.00	31.26	8
	ATOM	1300	N	ARG A 429	32.059	42.423	37.011	1.00	27.64	7
45	ATOM	1301	CA	ARG A 429	31.527	43.162	38.147	1.00	28.13	6
	ATOM	1302	CB	ARG A 429	32.564	43.298	39.264	1.00	29.59	6
	ATOM	1303	CG	ARG A 429	32.818	42.040	40.080	1.00	34.85	6
	ATOM	1304	CD	ARG A 429	33.588	42.360	41.367	1.00	47.18	6
	ATOM	1305	NE	ARG A 429	34.093	41.175	42.049	1.00	57.93	7
50	ATOM	1306	CZ	ARG A 429	33.327	40.210	42.547	1.00	63.62	6
	ATOM	1307	NH1	ARG A 429	31.998	40.270	42.396	1.00	60.71	7
	ATOM	1308	NH2	ARG A 429	33.900	39.165	43.150	1.00	62.38	7
	ATOM	1309	C	ARG A 429	31.099	44.536	37.707	1.00	29.81	6
	ATOM	1310	O	ARG A 429	30.044	45.009	38.101	1.00	30.81	8
55	ATOM	1311	N	MET A 430	31.941	45.176	36.901	1.00	29.64	7
	ATOM	1312	CA	MET A 430	31.644	46.502	36.383	1.00	34.72	6
	ATOM	1313	CB	MET A 430	32.745	46.955	35.434	1.00	34.97	6
	ATOM	1314	CG	MET A 430	33.937	47.597	36.080	1.00	45.34	6

5	ATOM	1315	SD	MET A 430	33.520	49.120	36.937	1.00	52.55	16
	ATOM	1316	CE	MET A 430	32.942	50.174	35.585	1.00	55.56	6
	ATOM	1317	C	MET A 430	30.315	46.455	35.634	1.00	34.01	6
	ATOM	1318	O	MET A 430	29.455	47.295	35.854	1.00	37.29	8
	ATOM	1319	N	ILE A 431	30.180	45.468	34.740	1.00	29.99	7
10	ATOM	1320	CA	ILE A 431	28.954	45.269	33.969	1.00	28.82	6
	ATOM	1321	CB	ILE A 431	28.962	43.936	33.211	1.00	27.39	6
	ATOM	1322	CG2	ILE A 431	27.622	43.671	32.572	1.00	23.87	6
	ATOM	1323	CG1	ILE A 431	30.044	43.920	32.138	1.00	25.56	6
	ATOM	1324	CD1	ILE A 431	29.989	42.703	31.244	1.00	17.29	6
15	ATOM	1325	C	ILE A 431	27.769	45.269	34.907	1.00	29.49	6
	ATOM	1326	O	ILE A 431	26.810	45.993	34.712	1.00	24.19	8
	ATOM	1327	N	GLY A 432	27.839	44.435	35.936	1.00	25.25	7
	ATOM	1328	CA	GLY A 432	26.748	44.343	36.890	1.00	30.38	6
	ATOM	1329	C	GLY A 432	26.494	45.671	37.554	1.00	32.75	6
20	ATOM	1330	O	GLY A 432	25.411	46.206	37.469	1.00	36.38	8
	ATOM	1331	N	ALA A 433	27.514	46.189	38.221	1.00	26.77	7
	ATOM	1332	CA	ALA A 433	27.428	47.459	38.910	1.00	26.48	6
	ATOM	1333	CB	ALA A 433	28.836	47.970	39.203	1.00	19.90	6
	ATOM	1334	C	ALA A 433	26.663	48.502	38.114	1.00	30.73	6
25	ATOM	1335	O	ALA A 433	25.773	49.164	38.635	1.00	31.60	8
	ATOM	1336	N	CYS A 434	27.027	48.654	36.854	1.00	33.22	7
	ATOM	1337	CA	CYS A 434	26.371	49.616	35.996	1.00	34.34	6
	ATOM	1338	CB	CYS A 434	27.047	49.612	34.711	1.00	35.20	6
	ATOM	1339	SG	CYS A 434	27.789	50.811	34.285	1.00	54.48	16
30	ATOM	1340	C	CYS A 434	24.974	49.198	35.612	1.00	34.09	6
	ATOM	1341	O	CYS A 434	24.107	50.040	35.415	1.00	34.89	8
	ATOM	1342	N	HIS A 435	24.756	47.898	35.447	1.00	34.30	7
	ATOM	1343	CA	HIS A 435	23.453	47.423	35.042	1.00	35.44	6
	ATOM	1344	CB	HIS A 435	23.404	45.904	35.104	1.00	31.76	6
35	ATOM	1345	CG	HIS A 435	22.099	45.351	34.675	1.00	32.03	6
	ATOM	1346	CD2	HIS A 435	21.697	44.790	33.519	1.00	28.61	6
	ATOM	1347	ND1	HIS A 435	20.941	45.482	35.452	1.00	28.48	7
	ATOM	1348	CE1	HIS A 435	19.912	45.025	34.759	1.00	33.27	6
	ATOM	1349	NE2	HIS A 435	20.345	44.597	33.583	1.00	31.57	7
40	ATOM	1350	C	HIS A 435	22.400	47.974	35.972	1.00	32.74	6
	ATOM	1351	O	HIS A 435	21.304	48.284	35.565	1.00	32.87	8
	ATOM	1352	N	ALA A 436	22.777	48.046	37.241	1.00	31.01	7
	ATOM	1353	CA	ALA A 436	21.910	48.563	38.266	1.00	29.91	6
	ATOM	1354	CB	ALA A 436	22.661	48.595	39.580	1.00	21.23	6
45	ATOM	1355	C	ALA A 436	21.475	49.969	37.884	1.00	33.86	6
	ATOM	1356	O	ALA A 436	20.296	50.298	37.910	1.00	36.10	8
	ATOM	1357	N	SER A 437	22.453	50.795	37.532	1.00	35.19	7
	ATOM	1358	CA	SER A 437	22.172	52.167	37.140	1.00	33.03	6
	ATOM	1359	CB	SER A 437	23.441	52.815	36.603	1.00	35.31	6
50	ATOM	1360	OG	SER A 437	23.203	54.151	36.193	1.00	44.99	8
	ATOM	1361	C	SER A 437	21.110	52.158	36.055	1.00	38.39	6
	ATOM	1362	O	SER A 437	20.049	52.745	36.204	1.00	37.54	8
	ATOM	1363	N	ARG A 438	21.432	51.483	34.956	1.00	37.32	7
	ATOM	1364	CA	ARG A 438	20.534	51.379	33.821	1.00	39.30	6
55	ATOM	1365	CB	ARG A 438	21.114	50.402	32.786	1.00	42.97	6
	ATOM	1366	CG	ARG A 438	22.343	50.911	32.051	1.00	41.72	6
	ATOM	1367	CD	ARG A 438	21.955	52.134	31.251	1.00	45.23	6
	ATOM	1368	NE	ARG A 438	20.964	51.839	30.237	1.00	45.66	7

5	ATOM	1369	CZ	ARG	A	438	20.063	52.718	30.318	1.00	50.91	6
	ATOM	1370	NH1	ARG	A	438	20.046	53.958	30.318	1.00	50.91	7
	ATOM	1371	NH2	ARG	A	438	19.198	52.354	28.865	1.00	46.86	7
	ATOM	1372	C	ARG	A	438	19.147	50.922	34.240	1.00	42.37	6
	ATOM	1373	O	ARG	A	438	18.147	51.297	33.625	1.00	40.58	8
10	ATOM	1374	N	PHE	A	439	19.080	50.120	35.298	1.00	42.25	7
	ATOM	1375	CA	PHE	A	439	17.803	49.624	35.763	1.00	42.81	6
	ATOM	1376	CB	PHE	A	439	17.975	48.794	37.013	1.00	42.18	6
	ATOM	1377	CG	PHE	A	439	16.739	48.053	37.413	1.00	42.48	6
	ATOM	1378	CD1	PHE	A	439	16.198	47.111	36.562	1.00	47.09	6
15	ATOM	1379	CD2	PHE	A	439	16.105	48.320	38.613	1.00	39.76	6
	ATOM	1380	CE1	PHE	A	439	15.047	46.427	36.905	1.00	49.17	6
	ATOM	1381	CE2	PHE	A	439	14.940	47.630	38.963	1.00	45.10	6
	ATOM	1382	CZ	PHE	A	439	14.411	46.683	38.098	1.00	46.36	6
	ATOM	1383	C	PHE	A	439	16.921	50.803	36.075	1.00	44.79	6
20	ATOM	1384	O	PHE	A	439	15.830	50.903	35.554	1.00	40.26	8
	ATOM	1385	N	LEU	A	440	17.410	51.681	36.951	1.00	42.77	7
	ATOM	1386	CA	LEU	A	440	16.660	52.871	37.344	1.00	42.96	6
	ATOM	1387	CB	LEU	A	440	17.546	53.824	38.150	1.00	37.19	6
	ATOM	1388	CG	LEU	A	440	17.943	53.297	39.500	1.00	36.97	6
25	ATOM	1389	CD1	LEU	A	440	18.620	54.389	40.316	1.00	33.65	6
	ATOM	1390	CD2	LEU	A	440	16.679	52.837	40.216	1.00	35.42	6
	ATOM	1391	C	LEU	A	440	16.025	53.596	36.168	1.00	45.47	6
	ATOM	1392	O	LEU	A	440	14.809	53.750	36.126	1.00	52.48	8
	ATOM	1393	N	HIS	A	441	16.836	54.060	35.223	1.00	49.15	7
30	ATOM	1394	CA	HIS	A	441	16.277	54.725	34.063	1.00	54.76	6
	ATOM	1395	CB	HIS	A	441	17.329	54.955	33.031	1.00	56.68	6
	ATOM	1396	CG	HIS	A	441	18.134	56.161	33.282	1.00	62.73	6
	ATOM	1397	CD2	HIS	A	441	18.468	57.216	32.499	1.00	65.73	6
	ATOM	1398	ND1	HIS	A	441	18.701	56.431	34.538	1.00	66.01	7
35	ATOM	1399	CE1	HIS	A	441	19.332	57.594	34.473	1.00	65.55	6
	ATOM	1400	NE2	HIS	A	441	19.205	58.085	33.255	1.00	60.09	7
	ATOM	1401	C	HIS	A	441	15.244	53.822	33.481	1.00	55.93	6
	ATOM	1402	O	HIS	A	441	14.149	54.263	33.170	1.00	57.33	8
	ATOM	1403	N	MET	A	442	15.605	52.549	33.313	1.00	57.81	7
40	ATOM	1404	CA	MET	A	442	14.661	51.583	32.778	1.00	59.11	6
	ATOM	1405	CB	MET	A	442	15.191	50.154	32.922	1.00	55.93	6
	ATOM	1406	CG	MET	A	442	16.336	49.813	32.022	1.00	58.52	6
	ATOM	1407	SD	MET	A	442	16.681	48.008	31.851	1.00	60.99	16
	ATOM	1408	CE	MET	A	442	17.085	47.602	33.581	1.00	52.61	6
45	ATOM	1409	C	MET	A	442	13.339	51.727	33.534	1.00	60.31	6
	ATOM	1410	O	MET	A	442	12.266	51.560	32.968	1.00	58.18	8
	ATOM	1411	N	LYS	A	443	13.425	52.054	34.818	1.00	61.45	7
	ATOM	1412	CA	LYS	A	443	12.236	52.202	35.626	1.00	64.90	6
	ATOM	1413	CB	LYS	A	443	12.608	52.141	37.090	1.00	64.40	6
50	ATOM	1414	CG	LYS	A	443	11.461	51.748	37.959	1.00	69.12	6
	ATOM	1415	CD	LYS	A	443	12.068	51.551	39.257	1.00	71.14	6
	ATOM	1416	CE	LYS	A	443	11.368	51.897	40.091	1.00	73.43	6
	ATOM	1417	NZ	LYS	A	443	11.883	51.712	41.415	1.00	67.97	7
	ATOM	1418	C	LYS	A	443	11.513	53.514	35.348	1.00	67.29	6
55	ATOM	1419	O	LYS	A	443	10.390	53.700	35.780	1.00	67.90	8
	ATOM	1420	N	VAL	A	444	12.171	54.429	34.629	1.00	66.57	7
	ATOM	1421	CA	VAL	A	444	11.575	55.719	34.297	1.00	64.76	6
	ATOM	1422	CB	VAL	A	444	12.569	56.869	34.560	1.00	62.76	6

5	ATOM	1423	CG1	VAL	A	444	11.952	58.195	34.173	1.00	64.183	6
	ATOM	1424	CG2	VAL	A	444	12.999	56.891	36.035	1.00	59.27	6
	ATOM	1425	C	VAL	A	444	11.043	55.730	32.861	1.00	68.61	6
	ATOM	1426	O	VAL	A	444	9.937	56.210	32.612	1.00	70.60	8
	ATOM	1427	N	GLU	A	445	11.814	55.173	31.935	1.00	70.71	7
10	ATOM	1428	CA	GLU	A	445	11.457	55.152	30.514	1.00	71.45	6
	ATOM	1429	CB	GLU	A	445	12.725	55.255	29.664	1.00	72.36	6
	ATOM	1430	CG	GLU	A	445	13.598	56.429	30.022	1.00	40.00	6
	ATOM	1431	CD	GLU	A	445	14.875	56.472	29.239	1.00	40.00	6
	ATOM	1432	OE1	GLU	A	445	15.155	55.565	28.414	1.00	40.00	8
15	ATOM	1433	OE2	GLU	A	445	15.663	57.430	29.430	1.00	40.00	8
	ATOM	1434	C	GLU	A	445	10.724	53.912	30.049	1.00	71.46	6
	ATOM	1435	O	GLU	A	445	10.536	53.701	28.844	1.00	73.02	8
	ATOM	1436	N	CYS	A	446	10.301	53.099	30.999	1.00	71.12	7
	ATOM	1437	CA	CYS	A	446	9.628	51.899	30.634	1.00	70.83	6
20	ATOM	1438	CB	CYS	A	446	10.595	50.719	30.687	1.00	71.05	6
	ATOM	1439	SG	CYS	A	446	12.009	50.842	29.573	1.00	72.83	16
	ATOM	1440	C	CYS	A	446	8.454	51.671	31.535	1.00	71.91	6
	ATOM	1441	O	CYS	A	446	8.495	52.014	32.728	1.00	72.06	8
	ATOM	1442	N	PRO	A	447	7.372	51.133	30.978	1.00	73.12	7
25	ATOM	1443	CD	PRO	A	447	7.267	50.764	29.560	1.00	72.88	6
	ATOM	1444	CA	PRO	A	447	6.150	50.853	31.740	1.00	74.22	6
	ATOM	1445	CB	PRO	A	447	5.187	50.281	30.714	1.00	72.98	6
	ATOM	1446	CG	PRO	A	447	5.875	50.271	29.437	1.00	74.77	6
	ATOM	1447	C	PRO	A	447	6.435	49.843	32.831	1.00	75.94	6
30	ATOM	1448	O	PRO	A	447	7.181	48.908	32.612	1.00	76.67	8
	ATOM	1449	N	THR	A	448	5.820	50.002	33.997	1.00	76.91	7
	ATOM	1450	CA	THR	A	448	6.024	49.066	35.113	1.00	78.24	6
	ATOM	1451	CB	THR	A	448	5.528	49.734	36.401	1.00	81.33	6
	ATOM	1452	OG1	THR	A	448	4.105	49.917	36.328	1.00	84.46	8
35	ATOM	1453	CG2	THR	A	448	6.192	51.081	36.585	1.00	83.51	6
	ATOM	1454	C	THR	A	448	5.113	47.912	34.755	1.00	77.42	6
	ATOM	1455	O	THR	A	448	4.915	46.995	35.519	1.00	77.65	8
	ATOM	1456	N	GLU	A	449	4.539	48.021	33.565	1.00	76.29	7
	ATOM	1457	CA	GLU	A	449	3.630	47.023	33.024	1.00	75.03	6
40	ATOM	1458	CB	GLU	A	449	2.600	47.773	32.191	1.00	74.62	6
	ATOM	1459	CG	GLU	A	449	2.145	47.051	31.001	1.00	40.00	6
	ATOM	1460	CD	GLU	A	449	1.297	47.889	30.178	1.00	40.00	6
	ATOM	1461	OE1	GLU	A	449	1.479	49.137	30.146	1.00	40.00	8
	ATOM	1462	OE2	GLU	A	449	0.424	47.322	29.497	1.00	40.00	8
45	ATOM	1463	C	GLU	A	449	4.434	46.036	32.179	1.00	73.49	6
	ATOM	1464	O	GLU	A	449	3.882	45.142	31.559	1.00	70.24	8
	ATOM	1465	N	LEU	A	450	5.747	46.224	32.161	1.00	70.80	7
	ATOM	1466	CA	LEU	A	450	6.608	45.347	31.378	1.00	68.82	6
	ATOM	1467	CB	LEU	A	450	7.301	46.154	30.277	1.00	71.91	6
50	ATOM	1468	CG	LEU	A	450	6.464	46.819	29.217	1.00	76.62	6
	ATOM	1469	CD1	LEU	A	450	7.337	47.662	28.328	1.00	77.95	6
	ATOM	1470	CD2	LEU	A	450	5.786	45.750	28.415	1.00	76.46	6
	ATOM	1471	C	LEU	A	450	7.669	44.673	32.243	1.00	66.22	6
	ATOM	1472	O	LEU	A	450	8.427	43.841	31.752	1.00	66.01	8
55	ATOM	1473	N	PHE	A	451	7.705	45.039	33.530	1.00	61.96	7
	ATOM	1474	CA	PHE	A	451	8.681	44.506	34.480	1.00	58.44	6
	ATOM	1475	CB	PHE	A	451	9.041	45.562	35.540	1.00	61.34	6
	ATOM	1476	CG	PHE	A	451	9.873	46.717	35.008	1.00	63.02	6

5	ATOM	1477	CD1	PHE	A	451	9.426	47.507	33.963	1.00	62.92	6
	ATOM	1478	CD2	PHE	A	451	11.089	47.017	35.593	1.00	63.07	6
	ATOM	1479	CE1	PHE	A	451	10.199	48.598	33.521	1.00	65.12	6
	ATOM	1480	CE2	PHE	A	451	11.860	48.102	35.156	1.00	64.66	6
	ATOM	1481	CZ	PHE	A	451	11.410	48.897	34.118	1.00	67.12	6
10	ATOM	1482	C	PHE	A	451	8.259	43.264	35.260	1.00	56.41	6
	ATOM	1483	O	PHE	A	451	7.641	43.392	36.331	1.00	56.56	8
	ATOM	1484	N	PRO	A	452	8.555	42.045	34.755	1.00	53.28	7
	ATOM	1485	CD	PRO	A	452	9.177	41.689	33.481	1.00	50.46	6
	ATOM	1486	CA	PRO	A	452	8.153	40.859	35.543	1.00	50.26	6
15	ATOM	1487	CB	PRO	A	452	8.739	39.680	34.780	1.00	49.19	6
	ATOM	1488	CG	PRO	A	452	9.178	40.206	33.482	1.00	45.89	6
	ATOM	1489	C	PRO	A	452	8.770	40.999	36.935	1.00	49.62	6
	ATOM	1490	O	PRO	A	452	9.867	41.529	37.094	1.00	52.35	8
	ATOM	1491	N	PRO	A	453	8.139	40.425	37.947	1.00	51.50	7
20	ATOM	1492	CD	PRO	A	453	7.001	39.542	37.797	1.00	49.66	6
	ATOM	1493	CA	PRO	A	453	8.610	40.528	39.323	1.00	50.89	6
	ATOM	1494	CB	PRO	A	453	7.675	39.659	40.109	1.00	51.49	6
	ATOM	1495	CG	PRO	A	453	6.703	39.141	39.185	1.00	50.82	6
	ATOM	1496	C	PRO	A	453	10.015	40.084	39.532	1.00	50.99	6
25	ATOM	1497	O	PRO	A	453	10.876	40.900	39.838	1.00	54.17	8
	ATOM	1498	N	LEU	A	454	10.255	38.781	39.423	1.00	51.21	7
	ATOM	1499	CA	LEU	A	454	11.585	38.298	39.674	1.00	47.17	6
	ATOM	1500	CB	LEU	A	454	11.813	36.962	38.975	1.00	44.44	6
	ATOM	1501	CG	LEU	A	454	13.167	36.375	39.289	1.00	41.33	6
30	ATOM	1502	CD1	LEU	A	454	13.524	36.638	40.720	1.00	35.93	6
	ATOM	1503	CD2	LEU	A	454	13.169	34.907	38.992	1.00	34.79	6
	ATOM	1504	C	LEU	A	454	12.541	39.375	39.182	1.00	42.25	6
	ATOM	1505	O	LEU	A	454	13.477	39.718	39.886	1.00	40.82	8
	ATOM	1506	N	PHE	A	455	12.270	39.957	38.011	1.00	39.29	7
35	ATOM	1507	CA	PHE	A	455	13.133	41.005	37.473	1.00	41.81	6
	ATOM	1508	CB	PHE	A	455	12.527	41.592	36.192	1.00	47.22	6
	ATOM	1509	CG	PHE	A	455	13.433	42.565	35.467	1.00	56.97	6
	ATOM	1510	CD1	PHE	A	455	14.715	42.189	35.135	1.00	57.23	6
	ATOM	1511	CD2	PHE	A	455	12.999	43.840	35.126	1.00	59.40	6
40	ATOM	1512	CE1	PHE	A	455	15.557	43.059	34.466	1.00	56.58	6
	ATOM	1513	CE2	PHE	A	455	13.848	44.716	34.452	1.00	61.80	6
	ATOM	1514	CZ	PHE	A	455	15.129	44.322	34.126	1.00	59.94	6
	ATOM	1515	C	PHE	A	455	13.273	42.085	38.534	1.00	45.12	6
	ATOM	1516	O	PHE	A	455	14.361	42.323	39.034	1.00	39.95	8
45	ATOM	1517	N	LEU	A	456	12.155	42.735	38.849	1.00	43.92	7
	ATOM	1518	CA	LEU	A	456	12.122	43.803	39.840	1.00	44.08	6
	ATOM	1519	CB	LEU	A	456	10.680	44.251	40.093	1.00	50.20	6
	ATOM	1520	CG	LEU	A	456	10.062	45.242	39.144	1.00	55.79	6
	ATOM	1521	CD1	LEU	A	456	8.598	45.432	39.450	1.00	54.70	6
50	ATOM	1522	CD2	LEU	A	456	10.807	46.548	39.295	1.00	53.01	6
	ATOM	1523	C	LEU	A	456	12.739	43.355	41.136	1.00	44.65	6
	ATOM	1524	O	LEU	A	456	13.597	44.022	41.685	1.00	45.93	8
	ATOM	1525	N	GLU	A	457	11.973	41.761	41.851	1.00	44.56	7
	ATOM	1526	CA	GLU	A	457	12.475	41.179	43.105	1.00	46.37	6
55	ATOM	1527	C	GLU	A	457	14.005	41.236	43.132	1.00	43.60	6
	ATOM	1528	O	GLU	A	457	14.583	41.724	44.117	1.00	42.69	8
	ATOM	1529	CB	GLU	A	457	12.024	39.723	43.223	1.00	50.16	6
	ATOM	1530	CG	GLU	A	457	11.114	39.476	44.427	1.00	20.00	6

5	ATOM	1531	CD	GLU	A	457	10.807	37.994	44.311	1.00	20.00	6
	ATOM	1532	OE1	GLU	A	457	11.673	37.099	44.311	1.00	20.00	8
	ATOM	1533	OE2	GLU	A	457	9.683	37.639	45.172	1.00	20.00	8
	ATOM	1534	N	VAL	A	458	14.928	41.078	41.903	1.00	43.21	7
	ATOM	1535	CA	VAL	A	458	16.412	41.094	41.868	1.00	44.98	6
10	ATOM	1536	CB	VAL	A	458	16.881	40.306	40.642	1.00	44.83	6
	ATOM	1537	CG1	VAL	A	458	18.365	40.106	40.698	1.00	49.72	6
	ATOM	1538	CG2	VAL	A	458	16.185	38.979	40.558	1.00	40.89	6
	ATOM	1539	C	VAL	A	458	17.130	42.420	41.877	1.00	42.72	6
	ATOM	1540	O	VAL	A	458	18.061	42.617	42.658	1.00	42.88	8
15	ATOM	1541	N	PHE	A	459	16.713	43.325	41.010	1.00	44.53	7
	ATOM	1542	CA	PHE	A	459	17.385	44.606	40.892	1.00	48.18	6
	ATOM	1543	CB	PHE	A	459	17.281	45.104	39.494	1.00	43.60	6
	ATOM	1544	CG	PHE	A	459	17.915	44.190	38.547	1.00	40.79	6
	ATOM	1545	CD1	PHE	A	459	17.325	42.983	38.244	1.00	41.01	6
20	ATOM	1546	CD2	PHE	A	459	19.153	44.483	38.054	1.00	39.48	6
	ATOM	1547	CE1	PHE	A	459	17.988	42.081	37.441	1.00	40.62	6
	ATOM	1548	CE2	PHE	A	459	19.814	43.589	37.257	1.00	36.87	6
	ATOM	1549	CZ	PHE	A	459	19.233	42.385	36.940	1.00	36.39	6
	ATOM	1550	C	PHE	A	459	16.837	45.648	41.744	1.00	52.71	6
25	ATOM	1551	O	PHE	A	459	17.492	46.682	42.017	1.00	51.34	8
	ATOM	1552	N	GLU	A	460	15.606	45.422	42.161	1.00	62.92	7
	ATOM	1553	CA	GLU	A	460	15.066	46.428	42.965	1.00	69.33	6
	ATOM	1554	CB	GLU	A	460	13.552	46.352	43.094	1.00	72.95	6
	ATOM	1555	CG	GLU	A	460	12.978	47.767	42.957	1.00	78.35	6
30	ATOM	1556	CD	GLU	A	460	12.246	48.261	44.157	1.00	82.97	6
	ATOM	1557	OE1	GLU	A	460	12.471	47.759	45.281	1.00	88.28	8
	ATOM	1558	OE2	GLU	A	460	11.422	49.200	44.017	1.00	84.80	8
	ATOM	1559	C	GLU	A	460	15.736	46.245	44.272	1.00	71.87	6
	ATOM	1560	O	GLU	A	460	16.187	45.170	44.691	1.00	74.51	8
35	ATOM	1561	N	ASP	A	461	15.790	47.373	44.917	1.00	78.50	7
	ATOM	1562	CA	ASP	A	461	16.415	47.505	46.173	1.00	84.19	6
	ATOM	1563	CB	ASP	A	461	16.394	48.981	46.471	1.00	85.82	6
	ATOM	1564	CG	ASP	A	461	16.801	49.786	45.276	1.00	89.62	6
	ATOM	1565	OD1	ASP	A	461	16.692	49.344	44.086	1.00	93.00	8
40	ATOM	1566	OD2	ASP	A	461	17.239	50.923	45.482	1.00	93.04	8
	ATOM	1567	C	ASP	A	461	15.639	46.703	47.214	1.00	86.80	6
	ATOM	1568	O	ASP	A	461	16.245	45.748	47.731	1.00	88.70	8
	ATOM	1569	OXT	ASP	A	461	14.457	47.026	47.451	1.00	88.70	8
	TER											
45	ATOM	1	CB	LYS	B	211	-20.802	66.251	39.780	1.00	46.72	6
	ATOM	2	CG	LYS	B	211	-19.566	65.345	39.922	1.00	56.48	6
	ATOM	3	CD	LYS	B	211	-18.264	66.114	40.045	1.00	60.93	6
	ATOM	4	CE	LYS	B	211	-18.043	67.067	38.886	1.00	61.95	6
	ATOM	5	NZ	LYS	B	211	-19.008	68.224	38.903	1.00	69.93	7
50	ATOM	6	C	LYS	B	211	-22.418	67.861	40.818	1.00	35.68	6
	ATOM	7	O	LYS	B	211	-23.356	67.113	40.454	1.00	33.58	8
	ATOM	8	N	LYS	B	211	-20.742	66.675	42.239	1.00	45.76	7
	ATOM	9	CA	LYS	B	211	-20.998	67.285	40.894	1.00	43.42	6
	ATOM	10	N	PRO	B	212	-22.610	69.205	41.068	1.00	35.64	7
55	ATOM	11	CD	PRO	B	212	-21.526	70.177	41.287	1.00	38.60	6
	ATOM	12	CA	PRO	B	212	-23.943	69.861	41.036	1.00	38.35	6
	ATOM	13	CB	PRO	B	212	-23.657	71.320	41.420	1.00	38.95	6
	ATOM	14	CG	PRO	B	212	-22.226	71.474	41.551	1.00	42.00	6

5	ATOM	15	C	PRO B 212	-24.798	69.772	39.807	1.00	38.78	6
	ATOM	16	O	PRO B 212	-24.350	70.045	38.696	1.00	34.64	8
	ATOM	17	N	GLU B 213	-26.058	69.424	40.032	1.00	40.31	7
	ATOM	18	CA	GLU B 213	-27.081	69.290	39.003	1.00	43.87	6
	ATOM	19	CB	GLU B 213	-27.895	68.004	39.265	1.00	45.16	6
10	ATOM	20	CG	GLU B 213	-27.032	66.709	39.286	1.00	47.60	6
	ATOM	21	CD	GLU B 213	-27.807	65.421	39.199	1.00	50.68	6
	ATOM	22	OE1	GLU B 213	-28.847	65.244	39.886	1.00	59.18	8
	ATOM	23	OE2	GLU B 213	-27.382	64.516	38.442	1.00	49.06	8
	ATOM	24	C	GLU B 213	-27.924	70.576	39.080	1.00	45.96	6
15	ATOM	25	O	GLU B 213	-27.624	71.467	39.859	1.00	43.13	8
	ATOM	26	N	PRO B 214	-28.987	70.698	38.308	1.00	46.52	7
	ATOM	27	CD	PRO B 214	-29.484	69.635	37.446	1.00	46.44	6
	ATOM	28	CA	PRO B 214	-29.843	71.907	38.302	1.00	47.52	6
	ATOM	29	CB	PRO B 214	-30.799	71.639	37.210	1.00	45.40	6
20	ATOM	30	CG	PRO B 214	-30.530	70.257	36.805	1.00	49.89	6
	ATOM	31	C	PRO B 214	-30.574	72.330	39.535	1.00	45.70	6
	ATOM	32	O	PRO B 214	-30.597	71.595	40.483	1.00	44.49	8
	ATOM	33	N	THR B 215	-31.180	73.515	39.506	1.00	45.24	7
	ATOM	34	CA	THR B 215	-31.965	74.036	40.652	1.00	49.36	6
25	ATOM	35	CB	THR B 215	-31.443	75.420	41.091	1.00	44.86	6
	ATOM	36	OG1	THR B 215	-32.249	76.464	40.534	1.00	52.26	8
	ATOM	37	CG2	THR B 215	-30.011	75.617	40.659	1.00	39.43	6
	ATOM	38	C	THR B 215	-33.386	74.239	40.114	1.00	52.51	6
	ATOM	39	O	THR B 215	-33.562	74.868	39.078	1.00	53.48	8
30	ATOM	40	N	ASP B 216	-34.387	73.741	40.829	1.00	58.81	7
	ATOM	41	CA	ASP B 216	-35.795	73.865	40.435	1.00	61.51	6
	ATOM	42	CB	ASP B 216	-36.674	74.005	41.650	1.00	70.57	6
	ATOM	43	CG	ASP B 216	-37.675	72.981	41.710	1.00	78.07	6
	ATOM	44	OD1	ASP B 216	-38.228	72.588	40.652	1.00	82.31	8
35	ATOM	45	OD2	ASP B 216	-37.983	72.567	42.830	1.00	86.55	8
	ATOM	46	C	ASP B 216	-35.920	75.123	39.648	1.00	58.42	6
	ATOM	47	O	ASP B 216	-36.847	75.317	38.827	1.00	56.85	8
	ATOM	48	N	GLU B 217	-34.954	75.979	39.984	1.00	54.92	7
	ATOM	49	CA	GLU B 217	-34.851	77.259	39.353	1.00	53.37	6
40	ATOM	50	CB	GLU B 217	-34.104	78.264	40.251	1.00	51.02	6
	ATOM	51	CG	GLU B 217	-34.151	79.689	39.679	1.00	40.00	6
	ATOM	52	CD	GLU B 217	-34.301	80.745	40.739	1.00	40.00	6
	ATOM	53	OE1	GLU B 217	-34.089	80.443	41.945	1.00	40.00	8
	ATOM	54	OE2	GLU B 217	-34.625	81.921	40.411	1.00	40.00	8
45	ATOM	55	C	GLU B 217	-34.232	77.163	37.957	1.00	53.55	6
	ATOM	56	O	GLU B 217	-34.815	77.612	37.018	1.00	54.33	8
	ATOM	57	N	GLU B 218	-33.063	76.572	37.839	1.00	49.20	7
	ATOM	58	CA	GLU B 218	-32.318	76.385	36.608	1.00	45.94	6
	ATOM	59	CB	GLU B 218	-30.965	75.793	36.981	1.00	43.43	6
50	ATOM	60	CG	GLU B 218	-30.065	76.728	37.801	1.00	40.86	6
	ATOM	61	CD	GLU B 218	-28.713	76.159	38.072	1.00	39.88	6
	ATOM	62	OE1	GLU B 218	-28.606	74.967	38.449	1.00	37.61	8
	ATOM	63	OE2	GLU B 218	-27.707	76.901	37.945	1.00	34.01	8
	ATOM	64	C	GLU B 218	-33.014	75.475	35.610	1.00	44.71	6
55	ATOM	65	O	GLU B 218	-32.935	75.686	34.405	1.00	45.31	8
	ATOM	66	N	TRP B 219	-33.669	74.439	36.131	1.00	44.02	7
	ATOM	67	CA	TRP B 219	-34.368	73.490	35.290	1.00	46.97	6
	ATOM	68	CB	TRP B 219	-35.046	72.408	36.119	1.00	48.42	6



5	ATOM	69	CG	TRP	B	219	-34.195	71.230	36.374	1.00	54.61	6
	ATOM	70	CD2	TRP	B	219	-34.048	70.120	35.478	1.00	55.24	6
	ATOM	71	CE2	TRP	B	219	-33.076	69.248	36.063	1.00	53.67	6
	ATOM	72	CE3	TRP	B	219	-34.615	69.771	34.252	1.00	54.55	6
	ATOM	73	CD1	TRP	B	219	-33.399	71.019	37.415	1.00	55.75	6
10	ATOM	74	NE1	TRP	B	219	-32.697	69.838	37.236	1.00	54.43	7
	ATOM	75	CZ2	TRP	B	219	-32.635	68.075	35.431	1.00	52.54	6
	ATOM	76	CZ3	TRP	B	219	-34.214	68.603	33.643	1.00	55.17	6
	ATOM	77	CH2	TRP	B	219	-33.234	67.758	34.214	1.00	55.59	6
	ATOM	78	C	TRP	B	219	-35.409	74.199	34.459	1.00	47.32	6
15	ATOM	79	O	TRP	B	219	-35.561	73.914	33.277	1.00	43.56	8
	ATOM	80	N	GLU	B	220	-36.126	75.130	35.084	1.00	49.91	7
	ATOM	81	CA	GLU	B	220	-37.158	75.874	34.402	1.00	53.57	6
	ATOM	82	CB	GLU	B	220	-37.811	76.820	35.373	1.00	58.18	6
	ATOM	83	CG	GLU	B	220	-39.251	76.812	35.221	1.00	73.13	6
20	ATOM	84	CD	GLU	B	220	-39.824	76.858	36.489	1.00	80.06	6
	ATOM	85	OE1	GLU	B	220	-39.485	75.995	37.324	1.00	82.12	8
	ATOM	86	OE2	GLU	B	220	-40.635	77.740	36.718	1.00	82.78	8
	ATOM	87	C	GLU	B	220	-36.539	76.645	33.250	1.00	50.51	6
	ATOM	88	O	GLU	B	220	-37.160	76.793	32.195	1.00	49.94	8
25	ATOM	89	N	LEU	B	221	-35.312	77.135	33.455	1.00	43.71	7
	ATOM	90	CA	LEU	B	221	-34.604	77.884	32.411	1.00	42.81	6
	ATOM	91	CB	LEU	B	221	-33.214	78.324	32.865	1.00	39.21	6
	ATOM	92	CG	LEU	B	221	-32.321	78.833	31.754	1.00	36.34	6
	ATOM	93	CD1	LEU	B	221	-33.073	79.843	30.927	1.00	36.93	6
30	ATOM	94	CD2	LEU	B	221	-31.058	79.446	32.331	1.00	24.18	6
	ATOM	95	C	LEU	B	221	-34.454	77.011	31.192	1.00	43.46	6
	ATOM	96	O	LEU	B	221	-34.819	77.406	30.104	1.00	45.25	8
	ATOM	97	N	ILE	B	222	-33.878	75.829	31.398	1.00	39.09	7
	ATOM	98	CA	ILE	B	222	-33.687	74.857	30.330	1.00	35.47	6
35	ATOM	99	CB	ILE	B	222	-33.224	73.516	30.871	1.00	33.74	6
	ATOM	100	CG2	ILE	B	222	-33.204	72.488	29.776	1.00	28.86	6
	ATOM	101	CG1	ILE	B	222	-31.840	73.631	31.493	1.00	33.33	6
	ATOM	102	CD1	ILE	B	222	-31.435	72.419	32.264	1.00	34.85	6
	ATOM	103	C	ILE	B	222	-34.991	74.627	29.598	1.00	34.26	6
40	ATOM	104	O	ILE	B	222	-35.082	74.832	28.392	1.00	31.90	8
	ATOM	105	N	LYS	B	223	-35.992	74.183	30.346	1.00	39.49	7
	ATOM	106	CA	LYS	B	223	-37.300	73.892	29.785	1.00	44.43	6
	ATOM	107	CB	LYS	B	223	-38.351	73.876	30.882	1.00	50.81	6
	ATOM	108	CG	LYS	B	223	-39.693	73.358	30.411	1.00	62.51	6
45	ATOM	109	CD	LYS	B	223	-40.795	73.532	31.449	1.00	72.22	6
	ATOM	110	CE	LYS	B	223	-42.163	73.249	30.827	1.00	74.55	6
	ATOM	111	NZ	LYS	B	223	-43.268	73.378	31.837	1.00	75.78	7
	ATOM	112	C	LYS	B	223	-37.648	74.942	28.755	1.00	42.81	6
	ATOM	113	O	LYS	B	223	-38.337	74.661	27.796	1.00	40.36	8
50	ATOM	114	N	THR	B	224	-37.146	76.156	28.979	1.00	39.89	7
	ATOM	115	CA	THR	B	224	-37.353	77.293	28.074	1.00	39.93	6
	ATOM	116	CB	THR	B	224	-36.956	78.609	28.776	1.00	40.57	6
	ATOM	117	OG1	THR	B	224	-37.646	78.740	30.028	1.00	39.27	8
	ATOM	118	CG2	THR	B	224	-37.273	79.805	27.893	1.00	38.11	6
55	ATOM	119	C	THR	B	224	-36.521	77.094	26.789	1.00	39.96	6
	ATOM	120	O	THR	B	224	-37.043	76.677	25.756	1.00	36.67	8
	ATOM	121	N	VAL	B	225	-35.231	77.421	26.888	1.00	38.02	7
	ATOM	122	CA	VAL	B	225	-34.263	77.295	25.801	1.00	38.12	6

5	ATOM	123	CB	VAL	B	225	-32.869	77.015	20.548	1.00	36.13	6
	ATOM	124	CG1	VAL	B	225	-31.863	76.983	25.226	1.00	36.77	6
	ATOM	125	CG2	VAL	B	225	-32.483	78.050	27.353	1.00	41.76	6
	ATOM	126	C	VAL	B	225	-34.656	76.191	24.843	1.00	37.52	6
	ATOM	127	O	VAL	B	225	-34.621	76.364	23.638	1.00	36.77	8
10	ATOM	128	N	THR	B	226	-35.005	75.046	25.410	1.00	34.02	7
	ATOM	129	CA	THR	B	226	-35.423	73.887	24.638	1.00	34.67	6
	ATOM	130	CB	THR	B	226	-35.677	72.707	25.574	1.00	30.56	6
	ATOM	131	OG1	THR	B	226	-34.432	72.225	26.084	1.00	32.20	8
	ATOM	132	CG2	THR	B	226	-36.413	71.595	24.874	1.00	20.99	6
15	ATOM	133	C	THR	B	226	-36.664	74.170	23.803	1.00	36.41	6
	ATOM	134	O	THR	B	226	-36.633	74.054	22.578	1.00	39.64	8
	ATOM	135	N	ALA	B	227	-37.746	74.542	24.480	1.00	39.20	7
	ATOM	136	CA	ALA	B	227	-39.008	74.861	23.822	1.00	36.93	6
	ATOM	137	CB	ALA	B	227	-39.914	75.631	24.785	1.00	38.06	6
20	ATOM	138	C	ALA	B	227	-38.686	75.719	22.608	1.00	37.69	6
	ATOM	139	O	ALA	B	227	-39.317	75.616	21.566	1.00	40.94	8
	ATOM	140	N	ALA	B	228	-37.677	76.572	22.785	1.00	32.86	7
	ATOM	141	CA	ALA	B	228	-37.216	77.483	21.753	1.00	32.48	6
	ATOM	142	CB	ALA	B	228	-36.252	78.458	22.358	1.00	28.25	6
25	ATOM	143	C	ALA	B	228	-36.545	76.704	20.638	1.00	36.12	6
	ATOM	144	O	ALA	B	228	-37.078	76.586	19.544	1.00	37.86	8
	ATOM	145	N	HIS	B	229	-35.364	76.175	20.924	1.00	33.58	7
	ATOM	146	CA	HIS	B	229	-34.611	75.409	19.956	1.00	32.97	6
	ATOM	147	CB	HIS	B	229	-33.418	74.721	20.597	1.00	33.69	6
30	ATOM	148	CG	HIS	B	229	-32.776	73.714	19.715	1.00	28.39	6
	ATOM	149	CD2	HIS	B	229	-32.535	72.384	19.863	1.00	28.83	6
	ATOM	150	ND1	HIS	B	229	-32.336	74.030	18.426	1.00	30.47	7
	ATOM	151	CE1	HIS	B	229	-31.867	72.929	17.855	1.00	26.95	6
	ATOM	152	NE2	HIS	B	229	-31.976	71.927	18.700	1.00	31.27	7
35	ATOM	153	C	HIS	B	229	-35.362	74.352	19.202	1.00	38.40	6
	ATOM	154	O	HIS	B	229	-35.069	74.131	18.045	1.00	41.49	8
	ATOM	155	N	VAL	B	230	-36.296	73.688	19.882	1.00	38.55	7
	ATOM	156	CA	VAL	B	230	-37.077	72.634	19.263	1.00	40.40	6
	ATOM	157	CB	VAL	B	230	-37.744	71.747	20.310	1.00	44.68	6
40	ATOM	158	CG1	VAL	B	230	-38.381	70.537	19.637	1.00	39.39	6
	ATOM	159	CG2	VAL	B	230	-36.742	71.311	21.356	1.00	42.18	6
	ATOM	160	C	VAL	B	230	-38.133	73.130	18.284	1.00	44.28	6
	ATOM	161	O	VAL	B	230	-38.375	72.505	17.248	1.00	45.94	8
	ATOM	162	N	ALA	B	231	-38.774	74.240	18.623	1.00	45.59	7
45	ATOM	163	CA	ALA	B	231	-39.820	74.804	17.792	1.00	47.84	6
	ATOM	164	CB	ALA	B	231	-40.736	75.661	18.647	1.00	45.08	6
	ATOM	165	C	ALA	B	231	-39.235	75.636	16.673	1.00	48.04	6
	ATOM	166	O	ALA	B	231	-39.959	76.128	15.816	1.00	49.95	8
	ATOM	167	N	THR	B	232	-37.914	75.773	16.669	1.00	47.26	7
50	ATOM	168	CA	THR	B	232	-37.220	76.563	15.654	1.00	43.64	6
	ATOM	169	CB	THR	B	232	-36.482	77.746	16.315	1.00	41.93	6
	ATOM	170	OG1	THR	B	232	-35.385	77.270	17.098	1.00	39.10	8
	ATOM	171	CG2	THR	B	232	-37.423	78.523	17.232	1.00	29.80	6
	ATOM	172	C	THR	B	232	-36.194	75.719	14.914	1.00	43.97	6
55	ATOM	173	O	THR	B	232	-35.401	76.252	14.155	1.00	40.55	8
	ATOM	174	N	ASN	B	233	-36.195	74.407	15.157	1.00	48.62	7
	ATOM	175	CA	ASN	B	233	-35.247	73.511	14.483	1.00	58.62	6
	ATOM	176	CB	ASN	B	233	-34.621	72.537	15.500	1.00	62.44	6

5	ATOM	177	CG	ASN	B	233	-33.407	71.812	14.256	1.00	68.33	6
	ATOM	178	OD1	ASN	B	233	-32.569	72.427	14.256	1.00	65.50	8
	ATOM	179	ND2	ASN	B	233	-33.288	70.529	15.265	1.00	74.29	7
	ATOM	180	C	ASN	B	233	-36.033	72.755	13.437	1.00	65.06	6
	ATOM	181	O	ASN	B	233	-36.950	72.005	13.754	1.00	69.47	8
10	ATOM	182	N	ALA	B	234	-35.674	72.986	12.182	1.00	68.80	7
	ATOM	183	CA	ALA	B	234	-36.352	72.376	11.036	1.00	70.98	6
	ATOM	184	CB	ALA	B	234	-35.585	72.701	9.769	1.00	71.43	6
	ATOM	185	C	ALA	B	234	-36.556	70.880	11.111	1.00	73.83	6
	ATOM	186	O	ALA	B	234	-35.677	70.142	11.501	1.00	74.33	8
15	ATOM	187	N	GLN	B	235	-37.754	70.479	10.717	1.00	75.07	7
	ATOM	188	CA	GLN	B	235	-38.149	69.095	10.690	1.00	76.32	6
	ATOM	189	CB	GLN	B	235	-37.468	68.365	9.533	1.00	76.98	6
	ATOM	190	CG	GLN	B	235	-38.120	68.540	8.170	1.00	77.07	6
	ATOM	191	CD	GLN	B	235	-38.572	69.940	7.909	1.00	80.85	6
20	ATOM	192	OE1	GLN	B	235	-39.575	70.401	8.491	1.00	82.01	8
	ATOM	193	NE2	GLN	B	235	-37.862	70.620	7.040	1.00	78.80	7
	ATOM	194	C	GLN	B	235	-37.904	68.331	11.953	1.00	77.15	6
	ATOM	195	O	GLN	B	235	-38.087	67.137	11.947	1.00	76.06	8
	ATOM	196	N	GLY	B	236	-37.511	68.985	13.039	1.00	77.46	7
25	ATOM	197	CA	GLY	B	236	-37.304	68.263	14.288	1.00	78.37	6
	ATOM	198	C	GLY	B	236	-36.717	66.882	14.217	1.00	79.43	6
	ATOM	199	O	GLY	B	236	-35.717	66.650	13.542	1.00	79.47	8
	ATOM	200	N	SER	B	237	-37.420	66.007	14.943	1.00	77.98	7
	ATOM	201	CA	SER	B	237	-37.117	64.600	15.092	1.00	76.49	6
30	ATOM	202	CB	SER	B	237	-38.118	63.953	16.066	1.00	76.46	6
	ATOM	203	C	SER	B	237	-37.181	63.895	13.737	1.00	75.35	6
	ATOM	204	O	SER	B	237	-36.493	62.911	13.524	1.00	75.47	8
	ATOM	205	N	HIS	B	238	-38.004	64.443	12.845	1.00	75.56	7
	ATOM	206	CA	HIS	B	238	-38.293	63.926	11.519	1.00	75.46	6
35	ATOM	207	CB	HIS	B	238	-39.663	64.397	11.096	1.00	75.85	6
	ATOM	208	C	HIS	B	238	-37.369	64.216	10.380	1.00	74.10	6
	ATOM	209	O	HIS	B	238	-37.747	64.135	9.222	1.00	75.34	8
	ATOM	210	N	TRP	B	239	-36.127	64.427	10.651	1.00	73.39	7
	ATOM	211	CA	TRP	B	239	-35.345	64.786	9.519	1.00	74.02	6
40	ATOM	212	CB	TRP	B	239	-34.121	65.542	9.934	1.00	81.77	6
	ATOM	213	CG	TRP	B	239	-33.085	64.786	10.737	1.00	89.67	6
	ATOM	214	CD2	TRP	B	239	-31.727	64.530	10.302	1.00	93.19	6
	ATOM	215	CE2	TRP	B	239	-31.069	63.848	11.393	1.00	95.46	6
	ATOM	216	CE3	TRP	B	239	-30.949	64.941	9.196	1.00	95.35	6
45	ATOM	217	CD1	TRP	B	239	-33.237	64.180	11.926	1.00	94.16	6
	ATOM	218	NE1	TRP	B	239	-32.022	63.631	12.347	1.00	97.48	7
	ATOM	219	CZ2	TRP	B	239	-29.706	63.475	11.348	1.00	96.23	6
	ATOM	220	CZ3	TRP	B	239	-29.613	64.533	9.128	1.00	96.75	6
	ATOM	221	CH2	TRP	B	239	-28.978	63.870	10.215	1.00	97.32	6
50	ATOM	222	C	TRP	B	239	-34.994	63.722	8.539	1.00	70.77	6
	ATOM	223	O	TRP	B	239	-35.423	63.772	7.388	1.00	71.70	8
	ATOM	224	N	LYS	B	240	-34.165	62.791	8.955	1.00	67.10	7
	ATOM	225	CA	LYS	B	240	-33.724	61.744	8.077	1.00	65.63	6
	ATOM	226	CB	LYS	B	240	-33.321	60.539	8.906	1.00	66.65	6
55	ATOM	227	CG	LYS	B	240	-32.210	60.824	9.905	1.00	69.83	6
	ATOM	228	CD	LYS	B	240	-31.759	59.553	10.602	1.00	71.49	6
	ATOM	229	CE	LYS	B	240	-30.576	59.843	11.493	1.00	71.31	6
	ATOM	230	NZ	LYS	B	240	-30.106	58.604	12.157	1.00	72.23	7

5	ATOM	231	C	LYS	B	240	-34.719	61.331	6.996	1.00	66.19	6
	ATOM	232	O	LYS	B	240	-34.321	60.673	6.031	1.00	65.20	8
	ATOM	233	N	ASN	B	241	-35.986	61.727	7.139	1.00	66.69	7
	ATOM	234	CA	ASN	B	241	-37.031	61.393	6.171	1.00	67.53	6
	ATOM	235	CB	ASN	B	241	-38.240	60.846	6.915	1.00	67.98	6
10	ATOM	236	CG	ASN	B	241	-37.966	59.479	7.544	1.00	70.19	6
	ATOM	237	OD1	ASN	B	241	-37.561	58.526	6.845	1.00	71.37	8
	ATOM	238	ND2	ASN	B	241	-38.205	59.370	8.836	1.00	71.48	7
	ATOM	239	C	ASN	B	241	-37.496	62.532	5.255	1.00	66.62	6
	ATOM	240	O	ASN	B	241	-38.504	62.395	4.578	1.00	64.76	8
15	ATOM	241	N	LYS	B	242	-36.753	63.633	5.209	1.00	66.86	7
	ATOM	242	CA	LYS	B	242	-37.096	64.772	4.362	1.00	67.46	6
	ATOM	243	CB	LYS	B	242	-37.501	65.948	5.258	1.00	67.93	6
	ATOM	244	CG	LYS	B	242	-38.746	65.684	6.076	1.00	71.52	6
	ATOM	245	CD	LYS	B	242	-40.007	65.528	5.215	1.00	74.32	6
20	ATOM	246	CE	LYS	B	242	-40.416	66.852	4.564	1.00	74.41	6
	ATOM	247	NZ	LYS	B	242	-40.657	67.941	5.575	1.00	74.44	7
	ATOM	248	C	LYS	B	242	-35.826	65.081	3.592	1.00	66.28	6
	ATOM	249	O	LYS	B	242	-35.814	65.799	2.601	1.00	67.61	8
	ATOM	250	N	ARG	B	243	-34.763	64.485	4.112	1.00	64.19	7
25	ATOM	251	CA	ARG	B	243	-33.410	64.577	3.591	1.00	62.43	6
	ATOM	252	CB	ARG	B	243	-32.599	63.547	4.390	1.00	60.12	6
	ATOM	253	CG	ARG	B	243	-31.128	63.558	4.171	1.00	40.00	6
	ATOM	254	CD	ARG	B	243	-30.335	62.888	5.319	1.00	40.00	6
	ATOM	255	NE	ARG	B	243	-30.269	61.428	5.296	1.00	40.00	7
30	ATOM	256	CZ	ARG	B	243	-29.384	60.724	6.009	1.00	40.00	6
	ATOM	257	NH1	ARG	B	243	-28.510	61.357	6.798	1.00	40.00	7
	ATOM	258	NH2	ARG	B	243	-29.355	59.401	5.908	1.00	40.00	7
	ATOM	259	C	ARG	B	243	-33.408	64.252	2.100	1.00	62.97	6
	ATOM	260	O	ARG	B	243	-33.690	63.122	1.722	1.00	63.96	8
35	ATOM	261	N	LYS	B	244	-33.105	65.245	1.270	1.00	62.41	7
	ATOM	262	CA	LYS	B	244	-33.054	65.053	-0.179	1.00	61.57	6
	ATOM	263	CB	LYS	B	244	-34.104	65.941	-0.866	1.00	63.68	6
	ATOM	264	CG	LYS	B	244	-35.527	65.731	-0.337	1.00	71.29	6
	ATOM	265	CD	LYS	B	244	-36.566	66.549	-1.107	1.00	73.83	6
40	ATOM	266	CE	LYS	B	244	-36.219	68.045	-1.138	1.00	74.71	6
	ATOM	267	NZ	LYS	B	244	-36.169	68.689	0.219	1.00	73.32	7
	ATOM	268	C	LYS	B	244	-31.658	65.402	-0.670	1.00	59.30	6
	ATOM	269	O	LYS	B	244	-31.317	66.570	-0.852	1.00	56.34	8
	ATOM	270	N	PHE	B	245	-30.858	64.359	-0.875	1.00	57.06	7
45	ATOM	271	CA	PHE	B	245	-29.462	64.525	-1.305	1.00	59.01	6
	ATOM	272	CB	PHE	B	245	-28.786	63.179	-1.478	1.00	59.62	6
	ATOM	273	CG	PHE	B	245	-28.991	62.288	-0.339	1.00	66.60	6
	ATOM	274	CD1	PHE	B	245	-30.200	61.669	-0.172	1.00	67.17	6
	ATOM	275	CD2	PHE	B	245	-28.012	62.117	0.593	1.00	69.25	6
50	ATOM	276	CE1	PHE	B	245	-30.404	60.882	0.911	1.00	69.92	6
	ATOM	277	CE2	PHE	B	245	-28.229	61.329	1.669	1.00	70.50	6
	ATOM	278	CZ	PHE	B	245	-29.418	60.714	1.830	1.00	70.89	6
	ATOM	279	C	PHE	B	245	-29.301	65.282	-2.592	1.00	60.68	6
	ATOM	280	O	PHE	B	245	-29.859	64.911	-3.619	1.00	62.37	8
55	ATOM	281	N	LEU	B	246	-28.495	66.336	-2.505	1.00	60.10	7
	ATOM	282	CA	LEU	B	246	-28.201	67.199	-3.631	1.00	59.44	6
	ATOM	283	CB	LEU	B	246	-27.248	68.332	-3.231	1.00	57.43	6
	ATOM	284	CG	LEU	B	246	-27.118	69.474	-4.207	1.00	54.41	6

5	ATOM	285	CD1	LEU	B	246	-28.481	70.137	<del>17.433</del>	<del>1.00</del>	<del>52.43</del>	6
	ATOM	286	CD2	LEU	B	246	-26.112	70.470	-3.719	1.00	51.69	6
	ATOM	287	C	LEU	B	246	-27.585	66.379	-4.740	1.00	62.05	6
	ATOM	288	O	LEU	B	246	-26.789	65.446	-4.486	1.00	59.85	8
	ATOM	289	N	PRO	B	247	-27.930	66.693	-5.984	1.00	63.33	7
10	ATOM	290	CD	PRO	B	247	-28.839	67.781	-6.363	1.00	64.44	6
	ATOM	291	CA	PRO	B	247	-27.391	65.958	-7.130	1.00	63.56	6
	ATOM	292	CB	PRO	B	247	-27.976	66.675	-8.340	1.00	64.42	6
	ATOM	293	CG	PRO	B	247	-28.873	67.714	-7.841	1.00	64.90	6
	ATOM	294	C	PRO	B	247	-25.866	65.947	-7.143	1.00	61.94	6
15	ATOM	295	O	PRO	B	247	-25.223	66.944	-6.856	1.00	61.60	8
	ATOM	296	N	GLU	B	248	-25.333	64.771	-7.478	1.00	61.33	7
	ATOM	297	CA	GLU	B	248	-23.896	64.516	-7.590	1.00	63.50	6
	ATOM	298	CB	GLU	B	248	-23.630	63.154	-8.248	1.00	66.94	6
	ATOM	299	CG	GLU	B	248	-22.168	62.953	-8.713	1.00	68.70	6
20	ATOM	300	CD	GLU	B	248	-21.898	61.745	-9.580	1.00	40.00	6
	ATOM	301	OE1	GLU	B	248	-22.863	61.007	-10.035	1.00	40.00	8
	ATOM	302	OE2	GLU	B	248	-20.709	61.460	-9.838	1.00	40.00	8
	ATOM	303	C	GLU	B	248	-23.158	65.571	-8.415	1.00	64.19	6
	ATOM	304	O	GLU	B	248	-22.056	65.975	-8.066	1.00	65.56	8
25	ATOM	305	N	ASP	B	249	-23.796	66.019	-9.498	1.00	64.36	7
	ATOM	306	CA	ASP	B	249	-23.254	66.994	-10.436	1.00	63.33	6
	ATOM	307	CB	ASP	B	249	-24.122	67.031	-11.698	1.00	62.97	6
	ATOM	308	CG	ASP	B	249	-25.437	67.715	-11.489	1.00	64.63	6
	ATOM	309	OD1	ASP	B	249	-26.235	67.285	-10.629	1.00	64.84	8
30	ATOM	310	OD2	ASP	B	249	-25.726	68.718	-12.189	1.00	66.52	8
	ATOM	311	C	ASP	B	249	-23.068	68.413	-9.960	1.00	64.31	6
	ATOM	312	O	ASP	B	249	-22.117	69.084	-10.355	1.00	64.73	8
	ATOM	313	N	ILE	B	250	-23.987	68.892	-9.136	1.00	63.09	7
	ATOM	314	CA	ILE	B	250	-23.921	70.281	-8.660	1.00	64.39	6
35	ATOM	315	CB	ILE	B	250	-25.124	70.575	-7.798	1.00	65.79	6
	ATOM	316	CG2	ILE	B	250	-25.559	72.041	-7.858	1.00	64.78	6
	ATOM	317	CG1	ILE	B	250	-26.348	69.752	-8.206	1.00	65.28	6
	ATOM	318	CD1	ILE	B	250	-27.671	70.444	-7.887	1.00	65.08	6
	ATOM	319	C	ILE	B	250	-22.815	70.488	-7.714	1.00	65.21	6
40	ATOM	320	O	ILE	B	250	-22.754	69.847	-6.656	1.00	64.05	8
	ATOM	321	N	GLY	B	251	-22.024	71.392	-8.103	1.00	65.48	7
	ATOM	322	CA	GLY	B	251	-20.873	71.721	-7.342	1.00	67.32	6
	ATOM	323	C	GLY	B	251	-19.808	70.806	-7.800	1.00	68.52	6
	ATOM	324	O	GLY	B	251	-19.791	70.548	-9.025	1.00	65.49	8
45	ATOM	325	N	GLN	B	252	-19.074	70.440	-6.799	1.00	72.26	7
	ATOM	326	CA	GLN	B	252	-17.949	69.540	-6.883	1.00	74.10	6
	ATOM	327	CB	GLN	B	252	-18.460	68.098	-6.723	1.00	75.82	6
	ATOM	328	CG	GLN	B	252	-17.367	67.088	-6.356	1.00	77.81	6
	ATOM	329	CD	GLN	B	252	-17.924	65.759	-5.824	1.00	79.38	6
50	ATOM	330	OE1	GLN	B	252	-18.615	65.042	-6.549	1.00	80.55	8
	ATOM	331	NE2	GLN	B	252	-17.661	65.380	-4.586	1.00	78.12	7
	ATOM	332	C	GLN	B	252	-17.258	69.727	-8.258	1.00	77.17	6
	ATOM	333	O	GLN	B	252	-17.977	70.009	-9.227	1.00	76.50	8
	ATOM	334	N	ALA	B	253	-15.718	69.795	-8.279	1.00	80.78	7
55	ATOM	335	CA	ALA	B	253	-14.615	70.766	-8.544	1.00	83.70	6
	ATOM	336	CB	ALA	B	253	-13.794	70.914	-7.255	1.00	83.23	6
	ATOM	337	C	ALA	B	253	-13.605	70.732	-9.731	1.00	85.59	6
	ATOM	338	O	ALA	B	253	-13.186	69.691	-10.171	1.00	85.69	8

5	ATOM	339	N	PRO B 254	-13.223	71.944	-11.121	1.00	33.05	7
	ATOM	340	CD	PRO B 254	-13.798	73.217	-9.752	1.00	33.97	6
	ATOM	341	CA	PRO B 254	-12.266	72.177	-11.351	1.00	35.89	6
	ATOM	342	CB	PRO B 254	-12.275	73.710	-11.596	1.00	33.94	6
	ATOM	343	CG	PRO B 254	-13.222	74.277	-10.688	1.00	33.31	6
10	ATOM	344	C	PRO B 254	-10.827	71.665	-11.121	1.00	37.75	6
	ATOM	345	O	PRO B 254	-10.379	71.426	-10.009	1.00	38.78	8
TER										
15	ATOM	1	N	GLY B 261	-8.238	79.356	-2.979	1.00	40.00	7
	ATOM	2	CA	GLY B 261	-9.314	78.411	-3.005	1.00	40.00	6
	ATOM	3	C	GLY B 261	-10.206	78.717	-4.355	1.00	40.00	6
	ATOM	4	O	GLY B 261	-11.372	79.141	-4.256	1.00	40.00	8
	ATOM	5	N	GLY B 262	-9.565	78.527	-5.597	1.00	40.00	7
20	ATOM	6	CA	GLY B 262	-10.136	78.609	-7.087	1.00	40.00	6
	ATOM	7	C	GLY B 262	-10.849	79.966	-7.577	1.00	40.00	6
	ATOM	8	O	GLY B 262	-10.200	81.044	-7.543	1.00	40.00	8
	ATOM	9	N	LYS B 263	-12.086	79.687	-8.124	1.00	61.71	7
	ATOM	10	CA	LYS B 263	-13.323	80.536	-8.428	1.00	64.36	6
25	ATOM	11	C	LYS B 263	-14.367	79.750	-7.614	1.00	63.41	6
	ATOM	12	O	LYS B 263	-14.102	78.579	-7.280	1.00	61.93	8
	ATOM	13	CB	LYS B 263	-13.901	80.405	-9.876	1.00	63.50	6
	ATOM	14	CG	LYS B 263	-13.487	81.474	-10.881	1.00	20.00	6
	ATOM	15	CD	LYS B 263	-14.016	82.897	-10.612	1.00	20.00	6
30	ATOM	16	CE	LYS B 263	-13.641	83.874	-11.742	1.00	20.00	6
	ATOM	17	NZ	LYS B 263	-13.680	85.287	-11.341	1.00	20.00	7
	ATOM	18	N	VAL B 264	-15.489	80.335	-7.307	1.00	61.15	7
	ATOM	19	CA	VAL B 264	-16.616	79.632	-6.619	1.00	59.46	6
	ATOM	20	CB	VAL B 264	-17.574	80.703	-6.099	1.00	59.03	6
35	ATOM	21	CG1	VAL B 264	-18.479	80.215	-4.979	1.00	53.79	6
	ATOM	22	CG2	VAL B 264	-16.847	81.938	-5.562	1.00	55.32	6
	ATOM	23	C	VAL B 264	-17.330	78.824	-7.700	1.00	60.96	6
	ATOM	24	O	VAL B 264	-16.940	78.873	-8.873	1.00	62.13	8
	ATOM	25	N	ASP B 265	-18.378	78.098	-7.340	1.00	62.59	7
40	ATOM	26	CA	ASP B 265	-19.175	77.339	-8.312	1.00	64.95	6
	ATOM	27	CB	ASP B 265	-18.796	75.851	-8.270	1.00	64.32	6
	ATOM	28	CG	ASP B 265	-19.928	75.022	-8.584	1.00	67.70	6
	ATOM	29	OD1	ASP B 265	-20.856	75.062	-9.295	1.00	72.59	8
	ATOM	30	OD2	ASP B 265	-20.370	73.959	-8.310	1.00	68.84	8
45	ATOM	31	C	ASP B 265	-20.658	77.614	-8.016	1.00	65.64	6
	ATOM	32	O	ASP B 265	-21.342	76.895	-7.313	1.00	68.81	8
	ATOM	33	N	LEU B 266	-21.066	78.737	-8.588	1.00	65.12	7
	ATOM	34	CA	LEU B 266	-22.385	79.330	-8.499	1.00	63.40	6
	ATOM	35	CB	LEU B 266	-22.429	80.448	-9.542	1.00	67.34	6
50	ATOM	36	CG	LEU B 266	-21.295	81.459	-9.399	1.00	69.35	6
	ATOM	37	CD1	LEU B 266	-20.983	82.127	-10.712	1.00	68.24	6
	ATOM	38	CD2	LEU B 266	-21.663	82.461	-8.344	1.00	70.47	6
	ATOM	39	C	LEU B 266	-23.673	78.507	-8.602	1.00	59.67	6
	ATOM	40	O	LEU B 266	-24.684	78.890	-7.988	1.00	53.35	8
55	ATOM	41	N	GLU B 267	-23.677	77.416	-9.371	1.00	58.01	7
	ATOM	42	CA	GLU B 267	-24.901	76.640	-9.449	1.00	58.34	6
	ATOM	43	CB	GLU B 267	-24.752	75.410	-10.368	1.00	59.21	6
	ATOM	44	CG	GLU B 267	-25.979	74.464	-10.268	1.00	62.89	6
	ATOM	45	CD	GLU B 267	-26.048	73.419	-11.328	1.00	67.66	6
	ATOM	46	OE1	GLU B 267	-25.076	72.645	-11.512	1.00	69.95	8

5	ATOM	47	OE2	GLU	B	267	-27.098	73.328	<del>-12.008</del>	1.00	69.40	8
	ATOM	48	C	GLU	B	267	-25.200	76.184	-8.032	1.00	57.67	6
	ATOM	49	O	GLU	B	267	-26.354	76.009	-7.643	1.00	58.34	8
	ATOM	50	N	ALA	B	268	-24.114	75.996	-7.285	1.00	53.43	7
	ATOM	51	CA	ALA	B	268	-24.151	75.560	-5.905	1.00	49.00	6
10	ATOM	52	CB	ALA	B	268	-22.816	74.956	-5.526	1.00	45.72	6
	ATOM	53	C	ALA	B	268	-24.421	76.775	-5.056	1.00	45.76	6
	ATOM	54	O	ALA	B	268	-25.419	76.823	-4.351	1.00	41.50	8
	ATOM	55	N	PHE	B	269	-23.533	77.766	-5.142	1.00	41.43	7
	ATOM	56	CA	PHE	B	269	-23.688	78.989	-4.358	1.00	43.96	6
15	ATOM	57	CB	PHE	B	269	-22.903	80.150	-4.971	1.00	40.10	6
	ATOM	58	CG	PHE	B	269	-23.057	81.458	-4.224	1.00	40.44	6
	ATOM	59	CD1	PHE	B	269	-22.284	81.727	-3.105	1.00	38.98	6
	ATOM	60	CD2	PHE	B	269	-24.033	82.372	-4.603	1.00	37.15	6
	ATOM	61	CE1	PHE	B	269	-22.472	82.921	-2.388	1.00	32.12	6
20	ATOM	62	CE2	PHE	B	269	-24.228	83.567	-3.890	1.00	38.41	6
	ATOM	63	CZ	PHE	B	269	-23.457	83.838	-2.780	1.00	40.55	6
	ATOM	64	C	PHE	B	269	-25.154	79.374	-4.320	1.00	49.76	6
	ATOM	65	O	PHE	B	269	-25.645	79.905	-3.336	1.00	52.15	8
	ATOM	66	N	SER	B	270	-25.840	79.112	-5.426	1.00	53.15	7
25	ATOM	67	CA	SER	B	270	-27.253	79.431	-5.520	1.00	52.29	6
	ATOM	68	CB	SER	B	270	-27.742	79.274	-6.948	1.00	51.85	6
	ATOM	69	OG	SER	B	270	-29.118	79.606	-7.048	1.00	53.42	8
	ATOM	70	C	SER	B	270	-28.012	78.486	-4.630	1.00	49.38	6
	ATOM	71	O	SER	B	270	-28.438	78.864	-3.548	1.00	48.74	8
30	ATOM	72	N	HIS	B	271	-28.185	77.253	-5.115	1.00	50.15	7
	ATOM	73	CA	HIS	B	271	-28.904	76.203	-4.382	1.00	51.67	6
	ATOM	74	CB	HIS	B	271	-28.409	74.812	-4.782	1.00	58.52	6
	ATOM	75	CG	HIS	B	271	-29.096	74.248	-5.976	1.00	68.97	6
	ATOM	76	CD2	HIS	B	271	-29.987	73.233	-6.102	1.00	70.88	6
35	ATOM	77	ND1	HIS	B	271	-28.943	74.770	-7.270	1.00	71.98	7
	ATOM	78	CE1	HIS	B	271	-29.716	74.080	-8.100	1.00	73.91	6
	ATOM	79	NE2	HIS	B	271	-30.354	73.149	-7.419	1.00	73.59	7
	ATOM	80	C	HIS	B	271	-28.785	76.347	-2.886	1.00	48.33	6
	ATOM	81	O	HIS	B	271	-29.641	75.874	-2.156	1.00	48.39	8
40	ATOM	82	N	PHE	B	272	-27.702	76.992	-2.444	1.00	41.34	7
	ATOM	83	CA	PHE	B	272	-27.440	77.224	-1.033	1.00	39.44	6
	ATOM	84	CB	PHE	B	272	-25.936	77.302	-0.801	1.00	36.67	6
	ATOM	85	CG	PHE	B	272	-25.241	75.945	-0.861	1.00	33.39	6
	ATOM	86	CD1	PHE	B	272	-23.856	75.857	-0.976	1.00	33.14	6
45	ATOM	87	CD2	PHE	B	272	-25.973	74.767	-0.732	1.00	38.28	6
	ATOM	88	CE1	PHE	B	272	-23.200	74.606	-0.989	1.00	38.26	6
	ATOM	89	CE2	PHE	B	272	-25.321	73.518	-0.743	1.00	43.28	6
	ATOM	90	CZ	PHE	B	272	-23.937	73.441	-0.856	1.00	39.74	6
	ATOM	91	C	PHE	B	272	-28.144	78.472	-0.477	1.00	40.75	6
50	ATOM	92	O	PHE	B	272	-28.803	78.393	0.558	1.00	35.51	8
	ATOM	93	N	THR	B	273	-28.027	79.621	-1.144	1.00	41.64	7
	ATOM	94	CA	THR	B	273	-28.658	80.850	-0.652	1.00	45.97	6
	ATOM	95	CB	THR	B	273	-28.023	82.105	-1.283	1.00	51.52	6
	ATOM	96	OG1	THR	B	273	-28.292	82.151	-2.688	1.00	45.74	8
55	ATOM	97	CG2	THR	B	273	-26.511	82.123	-1.048	1.00	49.73	6
	ATOM	98	C	THR	B	273	-30.142	80.859	-0.971	1.00	46.23	6
	ATOM	99	O	THR	B	273	-30.862	81.751	-0.535	1.00	41.21	8
	ATOM	100	N	LYS	B	274	-30.583	79.876	-1.758	1.00	46.21	7

5	ATOM	101	CA	LYS	B	274	-31.983	79.774	-2.147	1.00	54.53	6
	ATOM	102	CB	LYS	B	274	-32.133	78.724	-3.232	1.00	54.36	6
	ATOM	103	C	LYS	B	274	-32.819	79.396	-0.931	1.00	56.88	6
	ATOM	104	O	LYS	B	274	-34.025	79.624	-0.906	1.00	57.98	8
	ATOM	105	N	ILE	B	275	-32.151	78.820	0.076	1.00	56.48	7
10	ATOM	106	CA	ILE	B	275	-32.791	78.381	1.332	1.00	52.64	6
	ATOM	107	CB	ILE	B	275	-32.638	76.863	1.519	1.00	49.15	6
	ATOM	108	CG2	ILE	B	275	-33.505	76.105	0.529	1.00	47.42	6
	ATOM	109	CG1	ILE	B	275	-31.188	76.441	1.343	1.00	45.31	6
	ATOM	110	CD1	ILE	B	275	-30.990	74.952	1.391	1.00	37.22	6
15	ATOM	111	C	ILE	B	275	-32.241	79.086	2.574	1.00	51.78	6
	ATOM	112	O	ILE	B	275	-32.858	79.049	3.622	1.00	49.80	8
	ATOM	113	N	ILE	B	276	-31.071	79.709	2.435	1.00	51.76	7
	ATOM	114	CA	ILE	B	276	-30.410	80.409	3.533	1.00	52.58	6
	ATOM	115	CB	ILE	B	276	-29.145	81.110	3.042	1.00	55.04	6
20	ATOM	116	CG2	ILE	B	276	-29.486	82.172	2.017	1.00	53.28	6
	ATOM	117	CG1	ILE	B	276	-28.396	81.786	4.203	1.00	57.31	6
	ATOM	118	CD1	ILE	B	276	-27.862	80.854	5.231	1.00	60.32	6
	ATOM	119	C	ILE	B	276	-31.282	81.461	4.237	1.00	50.70	6
	ATOM	120	O	ILE	B	276	-31.015	81.817	5.385	1.00	55.55	8
25	ATOM	121	N	THR	B	277	-32.322	81.953	3.568	1.00	47.33	7
	ATOM	122	CA	THR	B	277	-33.174	82.968	4.141	1.00	42.59	6
	ATOM	123	CB	THR	B	277	-34.042	83.632	3.048	1.00	44.97	6
	ATOM	124	OG1	THR	B	277	-33.202	84.145	2.001	1.00	46.38	8
	ATOM	125	CG2	THR	B	277	-34.856	84.781	3.653	1.00	37.17	6
30	ATOM	126	C	THR	B	277	-34.069	82.447	5.267	1.00	39.84	6
	ATOM	127	O	THR	B	277	-34.083	83.026	6.375	1.00	40.55	8
	ATOM	128	N	PRO	B	278	-34.832	81.385	5.017	1.00	38.20	7
	ATOM	129	CD	PRO	B	278	-34.925	80.666	3.747	1.00	36.34	6
	ATOM	130	CA	PRO	B	278	-35.711	80.834	6.059	1.00	36.63	6
35	ATOM	131	CB	PRO	B	278	-36.475	79.715	5.357	1.00	32.95	6
	ATOM	132	CG	PRO	B	278	-35.833	79.516	4.056	1.00	35.75	6
	ATOM	133	C	PRO	B	278	-34.892	80.324	7.220	1.00	38.60	6
	ATOM	134	O	PRO	B	278	-35.372	80.157	8.331	1.00	37.67	8
	ATOM	135	N	ALA	B	279	-33.636	80.040	6.927	1.00	37.05	7
40	ATOM	136	CA	ALA	B	279	-32.696	79.525	7.903	1.00	33.18	6
	ATOM	137	CB	ALA	B	279	-31.391	79.195	7.205	1.00	30.56	6
	ATOM	138	C	ALA	B	279	-32.447	80.536	8.991	1.00	33.47	6
	ATOM	139	O	ALA	B	279	-32.623	80.238	10.158	1.00	33.74	8
	ATOM	140	N	ILE	B	280	-32.010	81.728	8.577	1.00	29.96	7
45	ATOM	141	CA	ILE	B	280	-31.728	82.809	9.501	1.00	25.94	6
	ATOM	142	CB	ILE	B	280	-31.190	84.040	8.754	1.00	26.95	6
	ATOM	143	CG2	ILE	B	280	-30.881	85.149	9.715	1.00	15.40	6
	ATOM	144	CG1	ILE	B	280	-29.904	83.696	8.007	1.00	26.73	6
	ATOM	145	CD1	ILE	B	280	-29.255	84.878	7.362	1.00	34.31	6
50	ATOM	146	C	ILE	B	280	-32.964	83.172	10.310	1.00	31.39	6
	ATOM	147	O	ILE	B	280	-32.882	83.378	11.522	1.00	35.69	8
	ATOM	148	N	THR	B	281	-34.113	83.233	9.647	1.00	30.90	7
	ATOM	149	CA	THR	B	281	-35.361	83.586	10.328	1.00	33.49	6
	ATOM	150	CB	THR	B	281	-36.598	83.396	9.419	1.00	37.18	6
55	ATOM	151	OG1	THR	B	281	-36.703	82.034	9.005	1.00	46.48	8
	ATOM	152	CG2	THR	B	281	-36.525	84.289	8.198	1.00	32.85	6
	ATOM	153	C	THR	B	281	-35.523	82.706	11.556	1.00	29.94	6
	ATOM	154	O	THR	B	281	-35.855	83.186	12.634	1.00	25.55	8



5	ATOM	155	N	ARG B 282	-35.296	81.405	11.378	1.00	32.70	7
	ATOM	156	CA	ARG B 282	-35.439	80.449	12.475	1.00	34.27	6
	ATOM	157	CB	ARG B 282	-34.999	79.060	12.020	1.00	33.78	6
	ATOM	158	CG	ARG B 282	-35.986	77.944	12.280	1.00	45.15	6
	ATOM	159	CD	ARG B 282	-36.701	77.514	11.015	1.00	58.24	6
10	ATOM	160	NE	ARG B 282	-35.771	77.153	9.969	1.00	68.41	7
	ATOM	161	CZ	ARG B 282	-34.862	76.200	10.098	1.00	72.31	6
	ATOM	162	NH1	ARG B 282	-34.779	75.502	11.232	1.00	77.89	7
	ATOM	163	NH2	ARG B 282	-34.022	75.963	9.096	1.00	69.25	7
	ATOM	164	C	ARG B 282	-34.556	80.919	13.622	1.00	34.81	6
15	ATOM	165	O	ARG B 282	-35.008	81.034	14.753	1.00	36.03	8
	ATOM	166	N	VAL B 283	-33.288	81.183	13.289	1.00	31.71	7
	ATOM	167	CA	VAL B 283	-32.304	81.667	14.249	1.00	30.16	6
	ATOM	168	CB	VAL B 283	-30.993	82.029	13.559	1.00	29.00	6
	ATOM	169	CG1	VAL B 283	-30.015	82.617	14.557	1.00	28.64	6
20	ATOM	170	CG2	VAL B 283	-30.385	80.816	12.915	1.00	28.28	6
	ATOM	171	C	VAL B 283	-32.848	82.884	14.994	1.00	32.50	6
	ATOM	172	O	VAL B 283	-32.619	83.057	16.185	1.00	33.48	8
	ATOM	173	N	VAL B 284	-33.573	83.728	14.265	1.00	30.96	7
	ATOM	174	CA	VAL B 284	-34.177	84.925	14.844	1.00	29.14	6
25	ATOM	175	CB	VAL B 284	-34.672	85.892	13.751	1.00	31.27	6
	ATOM	176	CG1	VAL B 284	-35.278	87.129	14.371	1.00	24.21	6
	ATOM	177	CG2	VAL B 284	-33.554	86.270	12.812	1.00	30.51	6
	ATOM	178	C	VAL B 284	-35.336	84.498	15.747	1.00	28.89	6
	ATOM	179	O	VAL B 284	-35.491	84.994	16.860	1.00	27.29	8
30	ATOM	180	N	ASP B 285	-36.143	83.564	15.250	1.00	28.76	7
	ATOM	181	CA	ASP B 285	-37.299	83.057	15.983	1.00	35.32	6
	ATOM	182	CB	ASP B 285	-38.129	82.098	15.111	1.00	33.29	6
	ATOM	183	CG	ASP B 285	-38.881	82.795	14.013	1.00	38.15	6
	ATOM	184	OD1	ASP B 285	-39.660	83.729	14.305	1.00	34.70	8
35	ATOM	185	OD2	ASP B 285	-38.741	82.406	12.821	1.00	34.43	8
	ATOM	186	C	ASP B 285	-36.863	82.339	17.257	1.00	36.70	6
	ATOM	187	O	ASP B 285	-37.606	82.304	18.237	1.00	37.96	8
	ATOM	188	N	PHE B 286	-35.663	81.755	17.235	1.00	35.96	7
	ATOM	189	CA	PHE B 286	-35.134	81.053	18.401	1.00	37.10	6
40	ATOM	190	CB	PHE B 286	-33.870	80.262	18.052	1.00	37.97	6
	ATOM	191	CG	PHE B 286	-33.079	79.818	19.258	1.00	36.50	6
	ATOM	192	CD1	PHE B 286	-33.704	79.168	20.294	1.00	36.75	6
	ATOM	193	CD2	PHE B 286	-31.721	80.063	19.343	1.00	33.83	6
	ATOM	194	CE1	PHE B 286	-32.987	78.769	21.401	1.00	39.55	6
45	ATOM	195	CE2	PHE B 286	-30.997	79.662	20.456	1.00	38.08	6
	ATOM	196	CZ	PHE B 286	-31.632	79.013	21.486	1.00	34.44	6
	ATOM	197	C	PHE B 286	-34.808	82.023	19.504	1.00	36.83	6
	ATOM	198	O	PHE B 286	-35.246	81.845	20.631	1.00	35.61	8
	ATOM	199	N	ALA B 287	-34.005	83.027	19.169	1.00	37.33	7
50	ATOM	200	CA	ALA B 287	-33.599	84.035	20.132	1.00	36.34	6
	ATOM	201	CB	ALA B 287	-32.644	85.008	19.469	1.00	36.40	6
	ATOM	202	C	ALA B 287	-34.831	84.769	20.657	1.00	38.76	6
	ATOM	203	O	ALA B 287	-34.882	85.193	21.814	1.00	41.98	8
	ATOM	204	N	LYS B 288	-35.820	84.912	19.779	1.00	38.28	7
55	ATOM	205	CA	LYS B 288	-37.066	85.584	20.112	1.00	45.26	6
	ATOM	206	CB	LYS B 288	-37.983	85.690	18.898	1.00	48.35	6
	ATOM	207	CG	LYS B 288	-37.577	86.756	17.916	1.00	51.43	6
	ATOM	208	CD	LYS B 288	-38.806	87.359	17.226	1.00	60.23	6

5	ATOM	209	CE	LYS	B	288	-39.680	86.308	16.564	1.00	62.81	6
	ATOM	210	NZ	LYS	B	288	-38.897	85.460	15.614	1.00	64.69	7
	ATOM	211	C	LYS	B	288	-37.846	84.901	21.191	1.00	43.31	6
	ATOM	212	O	LYS	B	288	-38.650	85.532	21.857	1.00	45.66	8
	ATOM	213	N	LYS	B	289	-37.618	83.604	21.345	1.00	41.70	7
10	ATOM	214	CA	LYS	B	289	-38.313	82.849	22.351	1.00	40.67	6
	ATOM	215	CB	LYS	B	289	-38.554	81.418	21.845	1.00	42.25	6
	ATOM	216	CG	LYS	B	289	-39.438	81.368	20.589	1.00	39.53	6
	ATOM	217	CD	LYS	B	289	-40.093	80.010	20.422	1.00	43.19	6
	ATOM	218	CE	LYS	B	289	-41.025	79.987	19.223	1.00	45.74	6
15	ATOM	219	NZ	LYS	B	289	-42.391	80.476	19.512	1.00	52.49	7
	ATOM	220	C	LYS	B	289	-37.555	82.871	23.668	1.00	41.50	6
	ATOM	221	O	LYS	B	289	-38.057	82.366	24.657	1.00	39.77	8
	ATOM	222	N	LEU	B	290	-36.365	83.482	23.661	1.00	40.68	7
	ATOM	223	CA	LEU	B	290	-35.539	83.599	24.854	1.00	39.33	6
20	ATOM	224	CB	LEU	B	290	-34.053	83.499	24.491	1.00	36.14	6
	ATOM	225	CG	LEU	B	290	-33.640	82.240	23.767	1.00	34.81	6
	ATOM	226	CD1	LEU	B	290	-32.147	82.255	23.523	1.00	29.07	6
	ATOM	227	CD2	LEU	B	290	-34.013	81.040	24.607	1.00	33.45	6
	ATOM	228	C	LEU	B	290	-35.832	84.915	25.577	1.00	40.08	6
25	ATOM	229	O	LEU	B	290	-35.479	86.006	25.088	1.00	42.00	8
	ATOM	230	N	PRO	B	291	-36.462	84.840	26.765	1.00	40.27	7
	ATOM	231	CD	PRO	B	291	-36.819	83.613	27.494	1.00	39.65	6
	ATOM	232	CA	PRO	B	291	-36.782	86.069	27.501	1.00	38.28	6
	ATOM	233	CB	PRO	B	291	-37.376	85.574	28.811	1.00	35.88	6
30	ATOM	234	CG	PRO	B	291	-37.549	84.110	28.695	1.00	34.19	6
	ATOM	235	C	PRO	B	291	-35.570	87.002	27.714	1.00	40.05	6
	ATOM	236	O	PRO	B	291	-35.625	88.197	27.403	1.00	41.33	8
	ATOM	237	N	MET	B	292	-34.474	86.476	28.258	1.00	40.59	7
	ATOM	238	CA	MET	B	292	-33.296	87.286	28.545	1.00	42.86	6
35	ATOM	239	CB	MET	B	292	-32.149	86.376	28.975	1.00	43.28	6
	ATOM	240	CG	MET	B	292	-32.553	85.302	29.970	1.00	50.35	6
	ATOM	241	SD	MET	B	292	-31.070	84.609	30.755	1.00	51.17	16
	ATOM	242	CE	MET	B	292	-31.797	83.212	31.701	1.00	54.63	6
	ATOM	243	C	MET	B	292	-32.895	88.077	27.315	1.00	41.05	6
40	ATOM	244	O	MET	B	292	-32.228	89.098	27.420	1.00	39.66	8
	ATOM	245	N	PHE	B	293	-33.322	87.604	26.143	1.00	39.30	7
	ATOM	246	CA	PHE	B	293	-33.017	88.271	24.878	1.00	40.92	6
	ATOM	247	CB	PHE	B	293	-33.296	87.329	23.707	1.00	40.98	6
	ATOM	248	CG	PHE	B	293	-32.937	87.909	22.365	1.00	42.78	6
45	ATOM	249	CD1	PHE	B	293	-31.653	88.354	22.120	1.00	44.40	6
	ATOM	250	CD2	PHE	B	293	-33.872	87.972	21.350	1.00	43.66	6
	ATOM	251	CE1	PHE	B	293	-31.306	88.869	20.872	1.00	39.83	6
	ATOM	252	CE2	PHE	B	293	-33.525	88.486	20.100	1.00	46.21	6
	ATOM	253	CZ	PHE	B	293	-32.239	88.926	19.859	1.00	45.18	6
50	ATOM	254	C	PHE	B	293	-33.873	89.518	24.744	1.00	45.54	6
	ATOM	255	O	PHE	B	293	-33.369	90.626	24.579	1.00	42.01	8
	ATOM	256	N	CYS	B	294	-35.181	89.305	24.808	1.00	47.05	7
	ATOM	257	CA	CYS	B	294	-36.146	90.382	24.689	1.00	50.15	6
	ATOM	258	CB	CYS	B	294	-37.553	89.793	24.756	1.00	45.90	6
55	ATOM	259	SG	CYS	B	294	-37.899	88.607	23.449	1.00	51.50	16
	ATOM	260	C	CYS	B	294	-35.974	91.474	25.751	1.00	51.38	6
	ATOM	261	O	CYS	B	294	-36.585	92.536	25.656	1.00	53.83	8
	ATOM	262	N	GLU	B	295	-35.137	91.200	26.753	1.00	49.72	7

5	ATOM	263	CA	GLU B 295	-34.839	92.159	27.816	1.00	52.53	6
	ATOM	264	CB	GLU B 295	-34.553	91.412	29.131	1.00	57.40	6
	ATOM	265	CG	GLU B 295	-35.811	90.978	29.874	1.00	69.63	6
	ATOM	266	CD	GLU B 295	-36.610	92.144	30.375	1.00	78.49	6
	ATOM	267	OE1	GLU B 295	-36.153	92.869	31.297	1.00	82.82	8
10	ATOM	268	OE2	GLU B 295	-37.730	92.385	29.860	1.00	85.30	8
	ATOM	269	C	GLU B 295	-33.629	93.009	27.415	1.00	48.54	6
	ATOM	270	O	GLU B 295	-32.981	93.627	28.260	1.00	49.82	8
	ATOM	271	N	LEU B 296	-33.374	93.030	26.109	1.00	43.79	7
	ATOM	272	CA	LEU B 296	-32.268	93.761	25.540	1.00	45.42	6
15	ATOM	273	CB	LEU B 296	-31.319	92.769	24.838	1.00	41.04	6
	ATOM	274	CG	LEU B 296	-30.735	91.631	25.662	1.00	42.74	6
	ATOM	275	CD1	LEU B 296	-30.354	90.478	24.764	1.00	40.99	6
	ATOM	276	CD2	LEU B 296	-29.559	92.119	26.468	1.00	39.44	6
	ATOM	277	C	LEU B 296	-32.760	94.779	24.522	1.00	45.56	6
20	ATOM	278	O	LEU B 296	-33.845	94.600	23.924	1.00	43.07	8
	ATOM	279	N	PRO B 297	-32.004	95.875	24.338	1.00	46.99	7
	ATOM	280	CD	PRO B 297	-30.740	96.123	25.046	1.00	47.12	6
	ATOM	281	CA	PRO B 297	-32.388	96.912	23.363	1.00	49.61	6
	ATOM	282	CB	PRO B 297	-31.294	97.973	23.494	1.00	49.91	6
25	ATOM	283	CG	PRO B 297	-30.302	97.477	24.545	1.00	51.28	6
	ATOM	284	C	PRO B 297	-32.263	96.273	21.913	1.00	49.59	6
	ATOM	285	O	PRO B 297	-31.441	95.340	21.685	1.00	51.66	8
	ATOM	286	N	CYS B 298	-33.035	96.667	20.854	1.00	51.02	7
	ATOM	287	CA	CYS B 298	-32.761	96.150	19.456	1.00	52.86	6
30	ATOM	288	CB	CYS B 298	-33.140	97.165	18.356	1.00	54.57	6
	ATOM	289	SG	CYS B 298	-34.884	97.085	17.836	1.00	67.87	16
	ATOM	290	C	CYS B 298	-31.385	96.330	19.127	1.00	48.51	6
	ATOM	291	O	CYS B 298	-30.579	95.506	18.744	1.00	49.58	8
	ATOM	292	N	GLU B 299	-31.107	97.447	19.230	1.00	44.17	7
35	ATOM	293	CA	GLU B 299	-29.989	97.645	18.718	1.00	47.57	6
	ATOM	294	CB	GLU B 299	-29.402	98.973	19.208	1.00	49.92	6
	ATOM	295	CG	GLU B 299	-29.944	100.187	18.433	1.00	59.30	6
	ATOM	296	CD	GLU B 299	-31.090	100.887	19.164	1.00	63.80	6
	ATOM	297	OE1	GLU B 299	-31.673	101.904	18.629	1.00	69.03	8
40	ATOM	298	OE2	GLU B 299	-31.473	100.458	20.319	1.00	67.10	8
	ATOM	299	C	GLU B 299	-28.993	96.533	18.987	1.00	46.57	6
	ATOM	300	O	GLU B 299	-28.200	96.179	18.111	1.00	44.65	8
	ATOM	301	N	ASP B 300	-29.045	95.989	20.203	1.00	45.17	7
	ATOM	302	CA	ASP B 300	-28.152	94.908	20.584	1.00	43.32	6
45	ATOM	303	CB	ASP B 300	-27.985	94.849	22.105	1.00	37.38	6
	ATOM	304	CG	ASP B 300	-27.239	96.016	22.650	1.00	36.23	6
	ATOM	305	OD1	ASP B 300	-26.208	96.421	22.052	1.00	35.87	8
	ATOM	306	OD2	ASP B 300	-27.661	96.543	23.716	1.00	40.14	8
	ATOM	307	C	ASP B 300	-28.721	93.591	20.071	1.00	42.81	6
50	ATOM	308	O	ASP B 300	-28.001	92.775	19.489	1.00	46.02	8
	ATOM	309	N	GLN B 301	-30.019	93.399	20.306	1.00	38.60	7
	ATOM	310	CA	GLN B 301	-30.712	92.197	19.858	1.00	40.00	6
	ATOM	311	CB	GLN B 301	-32.234	92.418	19.836	1.00	38.59	6
	ATOM	312	CG	GLN B 301	-32.908	92.380	21.187	1.00	40.26	6
55	ATOM	313	CD	GLN B 301	-34.401	92.583	21.083	1.00	44.15	6
	ATOM	314	OE1	GLN B 301	-34.859	93.637	20.589	1.00	45.73	8
	ATOM	315	NE2	GLN B 301	-35.165	91.602	21.544	1.00	46.13	7
	ATOM	316	C	GLN B 301	-30.237	91.830	18.455	1.00	41.64	6

5	ATOM	317	O	GLN	B	301	-30.162	90.662	18.100	1.00	45.02	8
	ATOM	318	N	ILE	B	302	-29.916	92.864	17.674	1.00	41.01	7
	ATOM	319	CA	ILE	B	302	-29.424	92.692	16.311	1.00	40.23	6
	ATOM	320	CB	ILE	B	302	-29.584	93.978	15.498	1.00	39.52	6
	ATOM	321	CG2	ILE	B	302	-29.034	93.792	14.100	1.00	31.98	6
10	ATOM	322	CG1	ILE	B	302	-31.059	94.385	15.416	1.00	40.77	6
	ATOM	323	CD1	ILE	B	302	-31.939	93.317	14.775	1.00	45.43	6
	ATOM	324	C	ILE	B	302	-27.966	92.260	16.342	1.00	38.58	6
	ATOM	325	O	ILE	B	302	-27.613	91.197	15.830	1.00	40.81	8
	ATOM	326	N	ILE	B	303	-27.128	93.111	16.933	1.00	37.50	7
15	ATOM	327	CA	ILE	B	303	-25.692	92.846	17.062	1.00	39.33	6
	ATOM	328	CB	ILE	B	303	-25.066	93.648	18.203	1.00	39.06	6
	ATOM	329	CG2	ILE	B	303	-23.566	93.405	18.257	1.00	36.19	6
	ATOM	330	CG1	ILE	B	303	-25.309	95.143	18.020	1.00	40.15	6
	ATOM	331	CD1	ILE	B	303	-24.816	95.966	19.173	1.00	36.93	6
20	ATOM	332	C	ILE	B	303	-25.470	91.365	17.323	1.00	36.49	6
	ATOM	333	O	ILE	B	303	-24.619	90.725	16.712	1.00	36.58	8
	ATOM	334	N	LEU	B	304	-26.244	90.843	18.266	1.00	32.91	7
	ATOM	335	CA	LEU	B	304	-26.194	89.433	18.633	1.00	27.55	6
	ATOM	336	CB	LEU	B	304	-27.172	89.182	19.793	1.00	22.35	6
25	ATOM	337	CG	LEU	B	304	-26.623	89.449	21.187	1.00	26.88	6
	ATOM	338	CD1	LEU	B	304	-25.540	90.495	21.136	1.00	24.82	6
	ATOM	339	CD2	LEU	B	304	-27.747	89.840	22.121	1.00	23.69	6
	ATOM	340	C	LEU	B	304	-26.505	88.547	17.425	1.00	28.05	6
	ATOM	341	O	LEU	B	304	-25.668	87.751	16.983	1.00	24.68	8
30	ATOM	342	N	LEU	B	305	-27.716	88.700	16.897	1.00	26.34	7
	ATOM	343	CA	LEU	B	305	-28.145	87.939	15.741	1.00	30.91	6
	ATOM	344	CB	LEU	B	305	-29.460	88.514	15.199	1.00	32.50	6
	ATOM	345	CG	LEU	B	305	-30.699	88.305	16.050	1.00	33.36	6
	ATOM	346	CD1	LEU	B	305	-31.938	88.839	15.342	1.00	33.87	6
35	ATOM	347	CD2	LEU	B	305	-30.863	86.812	16.298	1.00	31.72	6
	ATOM	348	C	LEU	B	305	-27.072	87.922	14.666	1.00	29.76	6
	ATOM	349	O	LEU	B	305	-26.687	86.860	14.202	1.00	29.33	8
	ATOM	350	N	LYS	B	306	-26.597	89.107	14.291	1.00	29.72	7
	ATOM	351	CA	LYS	B	306	-25.576	89.254	13.264	1.00	34.28	6
40	ATOM	352	CB	LYS	B	306	-25.224	90.732	13.077	1.00	35.98	6
	ATOM	353	CG	LYS	B	306	-26.350	91.581	12.494	1.00	43.35	6
	ATOM	354	CD	LYS	B	306	-25.852	92.987	12.182	1.00	51.50	6
	ATOM	355	CE	LYS	B	306	-24.706	92.932	11.190	1.00	53.26	6
	ATOM	356	NZ	LYS	B	306	-23.883	94.161	11.251	1.00	59.61	7
45	ATOM	357	C	LYS	B	306	-24.308	88.484	13.556	1.00	35.25	6
	ATOM	358	O	LYS	B	306	-23.681	87.917	12.653	1.00	33.95	8
	ATOM	359	N	GLY	B	307	-23.918	88.478	14.829	1.00	35.79	7
	ATOM	360	CA	GLY	B	307	-22.702	87.793	15.227	1.00	34.59	6
	ATOM	361	C	GLY	B	307	-22.811	86.291	15.383	1.00	33.80	6
50	ATOM	362	O	GLY	B	307	-21.944	85.564	14.895	1.00	31.59	8
	ATOM	363	N	CYS	B	308	-23.861	85.843	16.071	1.00	31.15	7
	ATOM	364	CA	CYS	B	308	-24.069	84.434	16.320	1.00	29.04	6
	ATOM	365	CB	CYS	B	308	-24.761	84.240	17.663	1.00	27.59	6
	ATOM	366	SG	CYS	B	308	-26.496	84.629	17.608	1.00	30.50	16
55	ATOM	367	C	CYS	B	308	-24.911	83.712	15.266	1.00	30.59	6
	ATOM	368	O	CYS	B	308	-25.088	82.499	15.365	1.00	33.77	8
	ATOM	369	N	CYS	B	309	-25.432	84.429	14.266	1.00	28.46	7
	ATOM	370	CA	CYS	B	309	-26.270	83.787	13.265	1.00	30.10	6

5	ATOM	371	CB	CYS	B	309	-26.706	84.761	12.194	1.00	33.43	6
	ATOM	372	SG	CYS	B	309	-27.875	84.011	11.089	1.00	35.20	16
	ATOM	373	C	CYS	B	309	-25.617	82.608	12.603	1.00	27.72	6
	ATOM	374	O	CYS	B	309	-26.170	81.518	12.610	1.00	27.69	8
	ATOM	375	N	MET	B	310	-24.447	82.829	12.011	1.00	26.15	7
10	ATOM	376	CA	MET	B	310	-23.737	81.748	11.352	1.00	26.06	6
	ATOM	377	CB	MET	B	310	-22.439	82.263	10.712	1.00	25.32	6
	ATOM	378	CG	MET	B	310	-21.584	81.157	10.080	1.00	24.08	6
	ATOM	379	SD	MET	B	310	-22.555	80.324	8.758	1.00	27.71	16
	ATOM	380	CE	MET	B	310	-21.549	78.826	8.427	1.00	28.50	6
15	ATOM	381	C	MET	B	310	-23.416	80.673	12.374	1.00	25.94	6
	ATOM	382	O	MET	B	310	-23.659	79.489	12.151	1.00	28.09	8
	ATOM	383	N	GLU	B	311	-22.865	81.117	13.500	1.00	25.39	7
	ATOM	384	CA	GLU	B	311	-22.466	80.231	14.576	1.00	27.03	6
	ATOM	385	CB	GLU	B	311	-22.036	81.048	15.797	1.00	24.39	6
20	ATOM	386	CG	GLU	B	311	-21.019	82.141	15.509	1.00	26.00	6
	ATOM	387	CD	GLU	B	311	-20.524	82.835	16.740	1.00	23.95	6
	ATOM	388	OE1	GLU	B	311	-21.321	83.108	17.668	1.00	19.72	8
	ATOM	389	OE2	GLU	B	311	-19.313	83.163	16.815	1.00	26.51	8
	ATOM	390	C	GLU	B	311	-23.582	79.264	14.964	1.00	27.51	6
25	ATOM	391	O	GLU	B	311	-23.347	78.068	15.093	1.00	29.67	8
	ATOM	392	N	ILE	B	312	-24.794	79.792	15.145	1.00	26.82	7
	ATOM	393	CA	ILE	B	312	-25.933	78.967	15.527	1.00	25.71	6
	ATOM	394	CB	ILE	B	312	-27.125	79.814	16.021	1.00	23.35	6
	ATOM	395	CG2	ILE	B	312	-28.327	78.933	16.276	1.00	20.27	6
30	ATOM	396	CG1	ILE	B	312	-26.771	80.541	17.325	1.00	20.88	6
	ATOM	397	CD1	ILE	B	312	-27.952	81.163	18.028	1.00	18.15	6
	ATOM	398	C	ILE	B	312	-26.370	78.072	14.392	1.00	27.91	6
	ATOM	399	O	ILE	B	312	-26.769	76.926	14.605	1.00	28.96	8
	ATOM	400	N	MET	B	313	-26.303	78.603	13.174	1.00	27.66	7
35	ATOM	401	CA	MET	B	313	-26.696	77.832	11.999	1.00	30.18	6
	ATOM	402	CB	MET	B	313	-26.696	78.691	10.734	1.00	36.89	6
	ATOM	403	CG	MET	B	313	-27.882	79.634	10.607	1.00	37.95	6
	ATOM	404	SD	MET	B	313	-28.238	80.275	8.907	1.00	42.38	16
	ATOM	405	CE	MET	B	313	-26.787	81.316	8.639	1.00	40.68	6
40	ATOM	406	C	MET	B	313	-25.791	76.632	11.808	1.00	27.43	6
	ATOM	407	O	MET	B	313	-26.258	75.501	11.893	1.00	28.61	8
	ATOM	408	N	SER	B	314	-24.508	76.882	11.549	1.00	24.88	7
	ATOM	409	CA	SER	B	314	-23.533	75.824	11.346	1.00	27.98	6
	ATOM	410	CB	SER	B	314	-22.150	76.441	11.165	1.00	29.64	6
45	ATOM	411	OG	SER	B	314	-21.844	77.316	12.227	1.00	43.44	8
	ATOM	412	C	SER	B	314	-23.514	74.774	12.465	1.00	22.30	6
	ATOM	413	O	SER	B	314	-23.279	73.592	12.199	1.00	24.18	8
	ATOM	414	N	LEU	B	315	-23.760	75.187	13.714	1.00	23.99	7
	ATOM	415	CA	LEU	B	315	-23.792	74.219	14.811	1.00	25.07	6
50	ATOM	416	CB	LEU	B	315	-24.095	74.869	16.169	1.00	19.11	6
	ATOM	417	CG	LEU	B	315	-24.507	73.860	17.234	1.00	20.39	6
	ATOM	418	CD1	LEU	B	315	-23.390	72.878	17.493	1.00	18.92	6
	ATOM	419	CD2	LEU	B	315	-24.895	74.560	18.514	1.00	12.93	6
	ATOM	420	C	LEU	B	315	-24.892	73.219	14.517	1.00	24.53	6
55	ATOM	421	O	LEU	B	315	-24.672	72.014	14.550	1.00	26.32	8
	ATOM	422	N	ARG	B	316	-26.079	73.762	14.254	1.00	28.18	7
	ATOM	423	CA	ARG	B	316	-27.278	72.996	13.971	1.00	27.54	6
	ATOM	424	CB	ARG	B	316	-28.432	73.941	13.651	1.00	27.39	6

					-28.823	74.857	14.809	1.00	22.00	6
5	ATOM	425	CG	ARG B 316	-30.074	75.657	14.451	1.00	18.78	6
	ATOM	426	CD	ARG B 316	-30.905	75.944	15.598	1.00	26.57	7
	ATOM	427	NE	ARG B 316	-32.166	76.337	15.489	1.00	30.81	6
	ATOM	428	CZ	ARG B 316	-32.686	76.535	14.280	1.00	33.71	7
	ATOM	429	NH1	ARG B 316	-32.900	76.542	16.581	1.00	33.13	7
10	ATOM	430	NH2	ARG B 316	-27.128	72.028	12.830	1.00	28.09	6
	ATOM	431	C	ARG B 316	-27.852	71.053	12.760	1.00	32.41	8
	ATOM	432	O	ARG B 316	-26.187	72.309	11.941	1.00	28.36	7
	ATOM	433	N	ALA B 317	-25.938	71.466	10.794	1.00	26.64	6
	ATOM	434	CA	ALA B 317	-25.337	72.300	9.675	1.00	22.93	6
15	ATOM	435	CB	ALA B 317	-24.998	70.327	11.150	1.00	28.35	6
	ATOM	436	C	ALA B 317	-25.223	69.187	10.773	1.00	32.10	8
	ATOM	437	O	ALA B 317	-23.941	70.659	11.882	1.00	29.12	7
	ATOM	438	N	ALA B 318	-22.957	69.682	12.299	1.00	27.50	6
	ATOM	439	CA	ALA B 318	-21.915	70.355	13.160	1.00	28.39	6
20	ATOM	440	CB	ALA B 318	-23.645	68.591	13.084	1.00	28.10	6
	ATOM	441	C	ALA B 318	-23.415	67.415	12.854	1.00	28.18	8
	ATOM	442	O	ALA B 318	-24.502	69.012	14.016	1.00	29.16	7
	ATOM	443	N	VAL B 319	-25.259	68.107	14.889	1.00	35.24	6
	ATOM	444	CA	VAL B 319	-26.228	68.897	15.765	1.00	27.34	6
25	ATOM	445	CB	VAL B 319	-25.576	70.149	16.246	1.00	29.96	6
	ATOM	446	CG1	VAL B 319	-27.505	69.212	15.022	1.00	31.70	6
	ATOM	447	CG2	VAL B 319	-26.066	67.146	14.043	1.00	40.01	6
	ATOM	448	C	VAL B 319	-26.701	66.250	14.578	1.00	42.70	8
	ATOM	449	O	VAL B 319	-26.025	67.353	12.723	1.00	38.64	7
30	ATOM	450	N	ARG B 320	-26.770	66.541	11.762	1.00	38.61	6
	ATOM	451	CA	ARG B 320	-27.838	67.409	11.123	1.00	37.26	6
	ATOM	452	CB	ARG B 320	-29.152	67.280	11.822	1.00	43.12	6
	ATOM	453	CG	ARG B 320	-30.145	68.340	11.387	1.00	50.79	6
	ATOM	454	CD	ARG B 320	-31.500	67.911	11.705	1.00	54.71	7
35	ATOM	455	NE	ARG B 320	-32.555	68.723	11.597	1.00	57.89	6
	ATOM	456	CZ	ARG B 320	-32.398	69.957	11.130	1.00	49.08	7
	ATOM	457	NH1	ARG B 320	-33.773	68.302	11.844	1.00	59.59	7
	ATOM	458	NH2	ARG B 320	-25.937	65.910	10.670	1.00	42.14	6
	ATOM	459	C	ARG B 320	-26.381	65.802	9.532	1.00	46.30	8
40	ATOM	460	O	ARG B 320	-24.734	65.488	11.022	1.00	42.04	7
	ATOM	461	N	TYR B 321	-23.858	64.848	10.063	1.00	42.70	6
	ATOM	462	CA	TYR B 321	-22.433	65.332	10.297	1.00	38.01	6
	ATOM	463	CB	TYR B 321	-21.393	64.396	9.756	1.00	37.94	6
	ATOM	464	CG	TYR B 321	-21.265	64.176	8.397	1.00	33.85	6
45	ATOM	465	CD1	TYR B 321	-20.333	63.258	7.912	1.00	34.49	6
	ATOM	466	CE1	TYR B 321	-20.583	63.683	10.613	1.00	28.03	6
	ATOM	467	CD2	TYR B 321	-19.658	62.769	10.134	1.00	32.69	6
	ATOM	468	CE2	TYR B 321	-19.532	62.551	8.781	1.00	35.18	6
	ATOM	469	CZ	TYR B 321	-18.616	61.661	8.292	1.00	39.48	8
50	ATOM	470	OH	TYR B 321	-23.897	63.347	10.234	1.00	45.51	6
	ATOM	471	C	TYR B 321	-23.560	62.857	11.292	1.00	48.02	8
	ATOM	472	O	TYR B 321	-24.317	62.642	9.188	1.00	44.56	7
	ATOM	473	N	ASP B 322	-24.391	61.170	9.182	1.00	45.86	6
	ATOM	474	CA	ASP B 322	-25.570	60.749	8.294	1.00	46.64	6
55	ATOM	475	CB	ASP B 322	-25.449	59.359	7.775	1.00	40.00	6
	ATOM	476	CG	ASP B 322	-24.388	58.737	7.986	1.00	40.00	8
	ATOM	477	OD1	ASP B 322	-26.414	58.862	7.117	1.00	40.00	8
	ATOM	478	OD2	ASP B 322						

5	ATOM	479	C	ASP	B	322	-23.044	60.659	8.682	1.00	45.82	6
	ATOM	480	O	ASP	B	322	-22.738	60.783	7.495	1.00	45.38	8
	ATOM	481	N	PRO	B	323	-22.242	60.005	9.549	1.00	46.53	7
	ATOM	482	CD	PRO	B	323	-22.594	59.676	10.934	1.00	47.16	6
	ATOM	483	CA	PRO	B	323	-20.910	59.487	9.162	1.00	46.63	6
10	ATOM	484	CB	PRO	B	323	-20.367	58.847	10.433	1.00	43.95	6
	ATOM	485	CG	PRO	B	323	-21.398	58.958	11.454	1.00	43.93	6
	ATOM	486	C	PRO	B	323	-20.933	58.489	8.017	1.00	48.34	6
	ATOM	487	O	PRO	B	323	-20.040	58.457	7.171	1.00	50.84	8
	ATOM	488	N	GLU	B	324	-21.951	57.631	8.022	1.00	52.39	7
15	ATOM	489	CA	GLU	B	324	-22.126	56.615	7.008	1.00	55.85	6
	ATOM	490	CB	GLU	B	324	-23.491	55.960	7.216	1.00	55.54	6
	ATOM	491	CG	GLU	B	324	-23.678	55.332	8.581	1.00	40.00	6
	ATOM	492	CD	GLU	B	324	-22.642	54.294	8.888	1.00	40.00	6
	ATOM	493	OE1	GLU	B	324	-21.796	53.979	8.000	1.00	40.00	8
20	ATOM	494	OE2	GLU	B	324	-22.645	53.751	10.029	1.00	40.00	8
	ATOM	495	C	GLU	B	324	-22.087	57.292	5.655	1.00	54.94	6
	ATOM	496	O	GLU	B	324	-21.144	57.149	4.896	1.00	59.81	8
	ATOM	497	N	SER	B	325	-23.165	58.022	5.389	1.00	52.95	7
	ATOM	498	CA	SER	B	325	-23.358	58.762	4.163	1.00	50.10	6
25	ATOM	499	CB	SER	B	325	-24.768	59.357	4.163	1.00	48.23	6
	ATOM	500	OG	SER	B	325	-25.051	59.976	5.403	1.00	48.71	8
	ATOM	501	C	SER	B	325	-22.324	59.861	3.964	1.00	50.61	6
	ATOM	502	O	SER	B	325	-21.956	60.176	2.848	1.00	52.19	8
	ATOM	503	N	GLU	B	326	-21.851	60.422	5.070	1.00	45.64	7
30	ATOM	504	CA	GLU	B	326	-20.854	61.476	5.050	1.00	43.35	6
	ATOM	505	CB	GLU	B	326	-19.602	61.022	4.277	1.00	42.74	6
	ATOM	506	CG	GLU	B	326	-18.880	59.814	4.876	1.00	50.32	6
	ATOM	507	CD	GLU	B	326	-17.576	59.524	4.207	1.00	56.34	6
	ATOM	508	OE1	GLU	B	326	-16.898	58.545	4.608	1.00	59.31	8
35	ATOM	509	OE2	GLU	B	326	-17.177	60.255	3.266	1.00	55.74	8
	ATOM	510	C	GLU	B	326	-21.401	62.731	4.418	1.00	40.23	6
	ATOM	511	O	GLU	B	326	-20.793	63.285	3.514	1.00	40.44	8
	ATOM	512	N	THR	B	327	-22.528	63.208	4.934	1.00	35.90	7
	ATOM	513	CA	THR	B	327	-23.163	64.418	4.401	1.00	37.29	6
40	ATOM	514	CB	THR	B	327	-24.146	64.052	3.285	1.00	37.63	6
	ATOM	515	OG1	THR	B	327	-25.172	63.199	3.803	1.00	38.12	8
	ATOM	516	CG2	THR	B	327	-23.445	63.342	2.130	1.00	39.90	6
	ATOM	517	C	THR	B	327	-23.961	65.125	5.473	1.00	39.49	6
	ATOM	518	O	THR	B	327	-24.645	64.473	6.264	1.00	40.50	8
45	ATOM	519	N	LEU	B	328	-23.909	66.454	5.473	1.00	36.64	7
	ATOM	520	CA	LEU	B	328	-24.675	67.239	6.447	1.00	37.73	6
	ATOM	521	CB	LEU	B	328	-24.061	68.637	6.620	1.00	37.78	6
	ATOM	522	CG	LEU	B	328	-22.586	68.750	6.931	1.00	36.26	6
	ATOM	523	CD1	LEU	B	328	-22.260	70.145	7.411	1.00	36.56	6
50	ATOM	524	CD2	LEU	B	328	-22.231	67.751	8.000	1.00	39.85	6
	ATOM	525	C	LEU	B	328	-26.090	67.344	5.897	1.00	37.27	6
	ATOM	526	O	LEU	B	328	-26.358	66.855	4.805	1.00	34.96	8
	ATOM	527	N	THR	B	329	-26.989	67.975	6.647	1.00	39.73	7
	ATOM	528	CA	THR	B	329	-28.369	68.132	6.215	1.00	40.81	6
55	ATOM	529	CB	THR	B	329	-29.279	67.135	6.918	1.00	42.67	6
	ATOM	530	OG1	THR	B	329	-28.799	65.809	6.686	1.00	42.52	8
	ATOM	531	CG2	THR	B	329	-30.702	67.255	6.375	1.00	43.52	6
	ATOM	532	C	THR	B	329	-28.853	69.529	6.498	1.00	44.31	6

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5	ATOM	533	O	THR B 329	-29.432	69.801	7.535	1.00	43.72	8
	ATOM	534	N	LEU B 330	-28.589	70.413	5.546	1.00	44.62	7
	ATOM	535	CA	LEU B 330	-28.983	71.812	5.658	1.00	45.09	6
	ATOM	536	CB	LEU B 330	-28.354	72.608	4.510	1.00	44.66	6
	ATOM	537	CG	LEU B 330	-26.847	72.735	4.539	1.00	51.06	6
10	ATOM	538	CD1	LEU B 330	-26.226	71.367	4.640	1.00	48.58	6
	ATOM	539	CD2	LEU B 330	-26.364	73.450	3.299	1.00	45.18	6
	ATOM	540	C	LEU B 330	-30.508	71.965	5.652	1.00	48.06	6
	ATOM	541	O	LEU B 330	-31.211	71.244	4.959	1.00	49.33	8
	ATOM	542	N	ASN B 331	-30.988	72.911	6.458	1.00	52.20	7
15	ATOM	543	CA	ASN B 331	-32.407	73.214	6.588	1.00	54.41	6
	ATOM	544	CB	ASN B 331	-32.870	74.013	5.370	1.00	54.94	6
	ATOM	545	CG	ASN B 331	-33.687	75.220	5.749	1.00	60.35	6
	ATOM	546	OD1	ASN B 331	-33.182	76.130	6.430	1.00	61.84	8
	ATOM	547	ND2	ASN B 331	-34.935	75.242	5.324	1.00	65.92	7
20	ATOM	548	C	ASN B 331	-33.251	71.959	6.731	1.00	58.00	6
	ATOM	549	O	ASN B 331	-34.464	72.000	6.579	1.00	60.17	8
	ATOM	550	N	GLY B 332	-32.596	70.846	7.054	1.00	58.45	7
	ATOM	551	CA	GLY B 332	-33.295	69.587	7.235	1.00	58.55	6
	ATOM	552	C	GLY B 332	-33.909	69.004	5.984	1.00	59.79	6
25	ATOM	553	O	GLY B 332	-34.609	68.000	6.065	1.00	61.32	8
	ATOM	554	N	GLU B 333	-33.639	69.628	4.838	1.00	60.28	7
	ATOM	555	CA	GLU B 333	-34.196	69.182	3.571	1.00	59.13	6
	ATOM	556	CB	GLU B 333	-34.966	70.323	2.885	1.00	62.40	6
	ATOM	557	CG	GLU B 333	-36.099	70.963	3.690	1.00	75.69	6
30	ATOM	558	CD	GLU B 333	-36.720	72.135	2.998	1.00	80.41	6
	ATOM	559	OE1	GLU B 333	-35.984	73.081	2.618	1.00	79.98	8
	ATOM	560	OE2	GLU B 333	-37.966	72.158	2.830	1.00	83.81	8
	ATOM	561	C	GLU B 333	-33.110	68.722	2.624	1.00	57.18	6
	ATOM	562	O	GLU B 333	-33.236	67.689	1.974	1.00	57.50	8
35	ATOM	563	N	MET B 334	-32.054	69.528	2.539	1.00	55.20	7
	ATOM	564	CA	MET B 334	-30.926	69.259	1.653	1.00	50.85	6
	ATOM	565	CB	MET B 334	-30.514	70.563	0.984	1.00	48.70	6
	ATOM	566	CG	MET B 334	-29.244	70.460	0.194	1.00	45.39	6
	ATOM	567	SD	MET B 334	-28.743	72.008	-0.624	1.00	44.56	16
40	ATOM	568	CE	MET B 334	-30.307	72.445	-1.503	1.00	45.25	6
	ATOM	569	C	MET B 334	-29.711	68.634	2.319	1.00	51.59	6
	ATOM	570	O	MET B 334	-29.185	69.161	3.291	1.00	52.52	8
	ATOM	571	N	ALA B 335	-29.270	67.515	1.758	1.00	51.00	7
	ATOM	572	CA	ALA B 335	-28.106	66.802	2.267	1.00	48.98	6
45	ATOM	573	CB	ALA B 335	-28.377	65.304	2.274	1.00	47.86	6
	ATOM	574	C	ALA B 335	-26.931	67.108	1.371	1.00	51.01	6
	ATOM	575	O	ALA B 335	-26.936	66.760	0.190	1.00	51.61	8
	ATOM	576	N	VAL B 336	-25.921	67.770	1.930	1.00	46.62	7
	ATOM	577	CA	VAL B 336	-24.730	68.142	1.152	1.00	42.35	6
50	ATOM	578	CB	VAL B 336	-24.466	69.635	1.258	1.00	42.41	6
	ATOM	579	CG1	VAL B 336	-25.695	70.418	0.860	1.00	42.00	6
	ATOM	580	CG2	VAL B 336	-24.018	70.004	2.642	1.00	40.32	6
	ATOM	581	C	VAL B 336	-23.493	67.390	1.611	1.00	45.33	6
	ATOM	582	O	VAL B 336	-23.464	66.775	2.681	1.00	47.42	8
55	ATOM	583	N	THR B 337	-22.461	67.478	0.781	1.00	41.60	7
	ATOM	584	CA	THR B 337	-21.172	66.818	1.041	1.00	39.69	6
	ATOM	585	CB	THR B 337	-20.720	66.011	-0.173	1.00	41.35	6
	ATOM	586	OG1	THR B 337	-20.273	66.887	-1.213	1.00	49.35	8



5	ATOM	587	CG2	THR	B	337	-21.869	65.175	-0.702	1.00	40.38	6
	ATOM	588	C	THR	B	337	-20.087	67.846	1.318	1.00	37.88	6
	ATOM	589	O	THR	B	337	-20.141	68.975	0.832	1.00	34.06	8
	ATOM	590	N	ARG	B	338	-19.097	67.417	2.095	1.00	37.61	7
	ATOM	591	CA	ARG	B	338	-17.942	68.241	2.442	1.00	38.68	6
10	ATOM	592	CB	ARG	B	338	-16.770	67.333	2.823	1.00	35.95	6
	ATOM	593	CG	ARG	B	338	-15.455	68.042	3.064	1.00	38.83	6
	ATOM	594	CD	ARG	B	338	-14.348	67.029	3.319	1.00	35.88	6
	ATOM	595	NE	ARG	B	338	-14.520	66.239	4.530	1.00	37.42	7
	ATOM	596	CZ	ARG	B	338	-14.274	66.669	5.766	1.00	30.20	6
15	ATOM	597	NH1	ARG	B	338	-13.794	67.892	5.973	1.00	27.98	7
	ATOM	598	NH2	ARG	B	338	-14.481	65.847	6.788	1.00	27.40	7
	ATOM	599	C	ARG	B	338	-17.581	69.075	1.229	1.00	38.09	6
	ATOM	600	O	ARG	B	338	-17.537	70.299	1.284	1.00	34.12	8
	ATOM	601	N	GLY	B	339	-17.345	68.383	0.117	1.00	41.25	7
20	ATOM	602	CA	GLY	B	339	-16.981	69.054	-1.119	1.00	41.35	6
	ATOM	603	C	GLY	B	339	-18.004	70.109	-1.460	1.00	41.23	6
	ATOM	604	O	GLY	B	339	-17.736	71.291	-1.330	1.00	38.30	8
	ATOM	605	N	GLN	B	340	-19.174	69.665	-1.909	1.00	38.58	7
	ATOM	606	CA	GLN	B	340	-20.258	70.564	-2.276	1.00	40.79	6
25	ATOM	607	CB	GLN	B	340	-21.596	69.843	-2.079	1.00	40.82	6
	ATOM	608	CG	GLN	B	340	-21.830	68.657	-3.029	1.00	41.10	6
	ATOM	609	CD	GLN	B	340	-23.154	67.937	-2.783	1.00	48.84	6
	ATOM	610	OE1	GLN	B	340	-23.353	67.313	-1.715	1.00	50.53	8
	ATOM	611	NE2	GLN	B	340	-24.050	68.015	-3.753	1.00	54.25	7
30	ATOM	612	C	GLN	B	340	-20.239	71.872	-1.475	1.00	41.50	6
	ATOM	613	O	GLN	B	340	-20.114	72.958	-2.032	1.00	42.72	8
	ATOM	614	N	LEU	B	341	-20.352	71.736	-0.156	1.00	42.00	7
	ATOM	615	CA	LEU	B	341	-20.375	72.879	0.746	1.00	38.10	6
	ATOM	616	CB	LEU	B	341	-20.401	72.419	2.201	1.00	36.66	6
35	ATOM	617	CG	LEU	B	341	-20.678	73.514	3.194	1.00	39.94	6
	ATOM	618	CD1	LEU	B	341	-22.088	74.038	2.936	1.00	34.98	6
	ATOM	619	CD2	LEU	B	341	-20.570	72.990	4.609	1.00	40.95	6
	ATOM	620	C	LEU	B	341	-19.170	73.763	0.543	1.00	36.37	6
	ATOM	621	O	LEU	B	341	-19.293	74.974	0.497	1.00	37.89	8
40	ATOM	622	N	LYS	B	342	-18.003	73.136	0.433	1.00	33.29	7
	ATOM	623	CA	LYS	B	342	-16.737	73.843	0.239	1.00	35.17	6
	ATOM	624	CB	LYS	B	342	-15.603	72.821	0.176	1.00	34.97	6
	ATOM	625	CG	LYS	B	342	-14.210	73.401	0.306	1.00	40.00	6
	ATOM	626	CD	LYS	B	342	-13.155	72.288	0.316	1.00	34.48	6
45	ATOM	627	CE	LYS	B	342	-11.775	72.809	0.755	1.00	37.54	6
	ATOM	628	NZ	LYS	B	342	-10.790	71.680	0.981	1.00	42.32	7
	ATOM	629	C	LYS	B	342	-16.744	74.685	-1.038	1.00	38.29	6
	ATOM	630	O	LYS	B	342	-16.725	75.911	-0.993	1.00	36.23	8
	ATOM	631	N	ASN	B	343	-16.760	73.990	-2.172	1.00	39.25	7
50	ATOM	632	CA	ASN	B	343	-16.762	74.609	-3.481	1.00	40.19	6
	ATOM	633	CB	ASN	B	343	-16.977	73.539	-4.551	1.00	37.96	6
	ATOM	634	CG	ASN	B	343	-16.178	72.272	-4.277	1.00	39.22	6
	ATOM	635	OD1	ASN	B	343	-14.938	72.313	-4.106	1.00	42.37	8
	ATOM	636	ND2	ASN	B	343	-16.877	71.144	-4.259	1.00	42.19	7
55	ATOM	637	C	ASN	B	343	-17.894	75.624	-3.547	1.00	40.12	6
	ATOM	638	O	ASN	B	343	-17.835	76.600	-4.284	1.00	36.01	8
	ATOM	639	N	GLY	B	344	-18.934	75.361	-2.756	1.00	40.95	7
	ATOM	640	CA	GLY	B	344	-20.101	76.220	-2.709	1.00	39.25	6

5	ATOM	641	C	GLY B 344	-19.867	77.636	-2.258	1.00	38.26	6
	ATOM	642	O	GLY B 344	-20.715	78.501	-2.484	1.00	35.69	8
	ATOM	643	N	GLY B 345	-18.724	77.871	-1.619	1.00	35.89	7
	ATOM	644	CA	GLY B 345	-18.426	79.209	-1.159	1.00	34.00	6
	ATOM	645	C	GLY B 345	-17.848	79.298	0.230	1.00	38.64	6
10	ATOM	646	O	GLY B 345	-17.216	80.303	0.573	1.00	38.14	8
	ATOM	647	N	LEU B 346	-18.071	78.266	1.041	1.00	39.52	7
	ATOM	648	CA	LEU B 346	-17.563	78.279	2.403	1.00	36.05	6
	ATOM	649	CB	LEU B 346	-18.311	77.256	3.269	1.00	35.72	6
	ATOM	650	CG	LEU B 346	-19.800	77.473	3.378	1.00	34.89	6
15	ATOM	651	CD1	LEU B 346	-20.322	76.678	4.554	1.00	44.09	6
	ATOM	652	CD2	LEU B 346	-20.086	78.937	3.612	1.00	34.84	6
	ATOM	653	C	LEU B 346	-16.079	78.018	2.445	1.00	33.52	6
	ATOM	654	O	LEU B 346	-15.392	78.387	3.394	1.00	35.58	8
	ATOM	655	N	GLY B 347	-15.586	77.388	1.385	1.00	30.47	7
20	ATOM	656	CA	GLY B 347	-14.174	77.078	1.305	1.00	33.01	6
	ATOM	657	C	GLY B 347	-13.768	76.214	2.477	1.00	30.72	6
	ATOM	658	O	GLY B 347	-14.433	75.243	2.808	1.00	30.89	8
	ATOM	659	N	VAL B 348	-12.647	76.585	3.087	1.00	31.30	7
	ATOM	660	CA	VAL B 348	-12.097	75.867	4.227	1.00	31.27	6
25	ATOM	661	CB	VAL B 348	-10.889	76.609	4.817	1.00	31.66	6
	ATOM	662	CG1	VAL B 348	-11.292	77.974	5.360	1.00	20.19	6
	ATOM	663	CG2	VAL B 348	-10.250	75.786	5.905	1.00	24.77	6
	ATOM	664	C	VAL B 348	-13.136	75.651	5.360	1.00	33.84	6
	ATOM	665	O	VAL B 348	-13.002	74.707	6.153	1.00	29.99	8
30	ATOM	666	N	VAL B 349	-14.157	76.518	5.449	1.00	33.31	7
	ATOM	667	CA	VAL B 349	-15.147	76.339	6.483	1.00	32.23	6
	ATOM	668	CB	VAL B 349	-16.226	77.393	6.476	1.00	32.59	6
	ATOM	669	CG1	VAL B 349	-17.342	76.979	7.399	1.00	33.68	6
	ATOM	670	CG2	VAL B 349	-15.667	78.703	6.959	1.00	32.30	6
35	ATOM	671	C	VAL B 349	-15.792	74.987	6.380	1.00	34.91	6
	ATOM	672	O	VAL B 349	-16.055	74.359	7.394	1.00	33.73	8
	ATOM	673	N	SER B 350	-16.054	74.507	5.176	1.00	32.81	7
	ATOM	674	CA	SER B 350	-16.695	73.215	5.100	1.00	30.10	6
	ATOM	675	CB	SER B 350	-16.772	72.697	3.684	1.00	24.95	6
40	ATOM	676	OG	SER B 350	-17.538	71.502	3.644	1.00	23.16	8
	ATOM	677	C	SER B 350	-15.910	72.254	5.942	1.00	31.59	6
	ATOM	678	O	SER B 350	-16.417	71.807	6.950	1.00	37.62	8
	ATOM	679	N	ASP B 351	-14.675	71.942	5.565	1.00	28.60	7
	ATOM	680	CA	ASP B 351	-13.905	71.010	6.378	1.00	29.82	6
45	ATOM	681	CB	ASP B 351	-12.419	71.139	6.050	1.00	27.49	6
	ATOM	682	CG	ASP B 351	-12.151	71.094	4.585	1.00	30.22	6
	ATOM	683	OD1	ASP B 351	-12.013	72.174	3.954	1.00	32.61	8
	ATOM	684	OD2	ASP B 351	-12.064	69.980	4.017	1.00	30.02	8
	ATOM	685	C	ASP B 351	-14.176	71.343	7.861	1.00	30.63	6
50	ATOM	686	O	ASP B 351	-14.458	70.474	8.681	1.00	29.54	8
	ATOM	687	N	ALA B 352	-14.111	72.629	8.177	1.00	25.33	7
	ATOM	688	CA	ALA B 352	-14.346	73.092	9.533	1.00	28.59	6
	ATOM	689	CB	ALA B 352	-14.252	74.606	9.572	1.00	20.95	6
	ATOM	690	C	ALA B 352	-15.690	72.630	10.086	1.00	29.69	6
55	ATOM	691	O	ALA B 352	-15.757	72.068	11.164	1.00	30.36	8
	ATOM	692	N	ILE B 353	-16.754	72.884	9.330	1.00	27.63	7
	ATOM	693	CA	ILE B 353	-18.096	72.506	9.729	1.00	27.55	6
	ATOM	694	CB	ILE B 353	-19.144	73.129	8.800	1.00	28.04	6

5	ATOM	695	CG2	ILE	B	353	-20.529	72.673	9.195	1.00	23.68	6
	ATOM	696	CG1	ILE	B	353	-19.108	74.657	8.869	1.00	27.33	6
	ATOM	697	CD1	ILE	B	353	-20.141	75.313	7.964	1.00	26.23	6
	ATOM	698	C	ILE	B	353	-18.309	71.002	9.775	1.00	30.88	6
	ATOM	699	O	ILE	B	353	-19.021	70.499	10.639	1.00	31.22	8
10	ATOM	700	N	PHE	B	354	-17.728	70.279	8.822	1.00	29.86	7
	ATOM	701	CA	PHE	B	354	-17.881	68.831	8.797	1.00	31.08	6
	ATOM	702	CB	PHE	B	354	-17.461	68.249	7.439	1.00	28.80	6
	ATOM	703	CG	PHE	B	354	-18.568	68.233	6.405	1.00	28.80	6
	ATOM	704	CD1	PHE	B	354	-19.031	69.403	5.833	1.00	30.96	6
15	ATOM	705	CD2	PHE	B	354	-19.150	67.027	6.034	1.00	29.45	6
	ATOM	706	CE1	PHE	B	354	-20.066	69.362	4.902	1.00	27.12	6
	ATOM	707	CE2	PHE	B	354	-20.186	66.978	5.104	1.00	25.19	6
	ATOM	708	CZ	PHE	B	354	-20.644	68.146	4.535	1.00	28.09	6
	ATOM	709	C	PHE	B	354	-17.041	68.223	9.913	1.00	29.17	6
20	ATOM	710	O	PHE	B	354	-17.544	67.429	10.700	1.00	32.62	8
	ATOM	711	N	ASP	B	355	-15.761	68.593	9.972	1.00	23.86	7
	ATOM	712	CA	ASP	B	355	-14.864	68.090	11.005	1.00	25.34	6
	ATOM	713	CB	ASP	B	355	-13.582	68.929	11.045	1.00	21.41	6
	ATOM	714	CG	ASP	B	355	-12.548	68.456	10.086	1.00	32.08	6
25	ATOM	715	OD1	ASP	B	355	-12.899	68.069	8.944	1.00	33.58	8
	ATOM	716	OD2	ASP	B	355	-11.345	68.477	10.450	1.00	33.20	8
	ATOM	717	C	ASP	B	355	-15.570	68.153	12.357	1.00	27.86	6
	ATOM	718	O	ASP	B	355	-15.430	67.257	13.182	1.00	32.42	8
	ATOM	719	N	LEU	B	356	-16.339	69.223	12.561	1.00	26.84	7
30	ATOM	720	CA	LEU	B	356	-17.085	69.400	13.803	1.00	28.66	6
	ATOM	721	CB	LEU	B	356	-17.832	70.742	13.800	1.00	25.37	6
	ATOM	722	CG	LEU	B	356	-18.655	71.091	15.023	1.00	27.61	6
	ATOM	723	CD1	LEU	B	356	-17.729	71.248	16.191	1.00	25.43	6
	ATOM	724	CD2	LEU	B	356	-19.430	72.363	14.808	1.00	27.49	6
35	ATOM	725	C	LEU	B	356	-18.084	68.260	13.883	1.00	30.44	6
	ATOM	726	O	LEU	B	356	-18.054	67.445	14.804	1.00	31.55	8
	ATOM	727	N	GLY	B	357	-18.972	68.214	12.891	1.00	32.69	7
	ATOM	728	CA	GLY	B	357	-20.001	67.186	12.846	1.00	29.87	6
	ATOM	729	C	GLY	B	357	-19.486	65.832	13.279	1.00	33.12	6
40	ATOM	730	O	GLY	B	357	-20.032	65.246	14.207	1.00	29.41	8
	ATOM	731	N	MET	B	358	-18.444	65.351	12.593	1.00	33.31	7
	ATOM	732	CA	MET	B	358	-17.834	64.066	12.902	1.00	35.87	6
	ATOM	733	CB	MET	B	358	-16.513	63.903	12.151	1.00	34.56	6
	ATOM	734	CG	MET	B	358	-16.649	63.908	10.657	1.00	46.43	6
45	ATOM	735	SD	MET	B	358	-15.094	63.597	9.751	1.00	42.13	16
	ATOM	736	CE	MET	B	358	-14.121	65.063	10.228	1.00	44.29	6
	ATOM	737	C	MET	B	358	-17.552	63.976	14.392	1.00	33.26	6
	ATOM	738	O	MET	B	358	-18.019	63.075	15.075	1.00	36.39	8
	ATOM	739	N	SER	B	359	-16.766	64.933	14.875	1.00	33.31	7
50	ATOM	740	CA	SER	B	359	-16.380	64.998	16.270	1.00	34.39	6
	ATOM	741	CB	SER	B	359	-15.724	66.339	16.541	1.00	30.84	6
	ATOM	742	OG	SER	B	359	-15.130	66.355	17.825	1.00	47.14	8
	ATOM	743	C	SER	B	359	-17.579	64.813	17.169	1.00	36.43	6
	ATOM	744	O	SER	B	359	-17.635	63.853	17.922	1.00	35.46	8
55	ATOM	745	N	LEU	B	360	-18.525	65.744	17.079	1.00	36.74	7
	ATOM	746	CA	LEU	B	360	-19.741	65.729	17.889	1.00	35.44	6
	ATOM	747	CB	LEU	B	360	-20.706	66.817	17.405	1.00	34.16	6
	ATOM	748	CG	LEU	B	360	-20.263	68.255	17.575	1.00	34.59	6

5	ATOM	749	CD1	LEU B 360	-21.394	69.181	17.212	1.00	33.53	6
	ATOM	750	CD2	LEU B 360	-19.869	68.486	19.010	1.00	31.69	6
	ATOM	751	C	LEU B 360	-20.464	64.397	17.924	1.00	38.72	6
	ATOM	752	O	LEU B 360	-21.021	64.011	18.958	1.00	38.29	8
10	ATOM	753	N	SER B 361	-20.466	63.708	16.791	1.00	40.96	7
	ATOM	754	CA	SER B 361	-21.106	62.416	16.721	1.00	45.67	6
	ATOM	755	CB	SER B 361	-20.532	61.630	15.551	1.00	46.45	6
	ATOM	756	OG	SER B 361	-20.750	62.314	14.322	1.00	51.81	8
15	ATOM	757	C	SER B 361	-20.895	61.638	18.018	1.00	44.49	6
	ATOM	758	O	SER B 361	-21.696	60.793	18.362	1.00	46.67	8
	ATOM	759	N	SER B 362	-19.811	61.953	18.726	1.00	41.44	7
	ATOM	760	CA	SER B 362	-19.453	61.309	19.972	1.00	42.13	6
20	ATOM	761	CB	SER B 362	-17.962	61.510	20.234	1.00	42.61	6
	ATOM	762	OG	SER B 362	-17.164	61.025	19.158	1.00	51.87	8
	ATOM	763	C	SER B 362	-20.228	61.812	21.174	1.00	38.41	6
	ATOM	764	O	SER B 362	-20.602	61.025	22.035	1.00	38.01	8
25	ATOM	765	N	PHE B 363	-20.455	63.123	21.228	1.00	34.55	7
	ATOM	766	CA	PHE B 363	-21.150	63.735	22.346	1.00	32.96	6
	ATOM	767	CB	PHE B 363	-21.006	65.245	22.285	1.00	31.99	6
	ATOM	768	CG	PHE B 363	-19.578	65.719	22.378	1.00	29.97	6
30	ATOM	769	CD1	PHE B 363	-19.286	67.058	22.447	1.00	30.61	6
	ATOM	770	CD2	PHE B 363	-18.536	64.800	22.391	1.00	32.02	6
	ATOM	771	CE1	PHE B 363	-17.966	67.489	22.543	1.00	33.67	6
	ATOM	772	CE2	PHE B 363	-17.221	65.222	22.484	1.00	30.91	6
35	ATOM	773	CZ	PHE B 363	-16.927	66.557	22.554	1.00	29.33	6
	ATOM	774	C	PHE B 363	-22.617	63.361	22.482	1.00	30.52	6
	ATOM	775	O	PHE B 363	-23.142	63.331	23.596	1.00	32.19	8
	ATOM	776	N	ASN B 364	-23.279	63.075	21.361	1.00	33.51	7
40	ATOM	777	CA	ASN B 364	-24.683	62.701	21.377	1.00	38.03	6
	ATOM	778	CB	ASN B 364	-24.855	61.369	22.111	1.00	42.32	6
	ATOM	779	CG	ASN B 364	-24.008	60.271	21.524	1.00	53.11	6
	ATOM	780	OD1	ASN B 364	-24.183	59.895	20.344	1.00	59.51	8
45	ATOM	781	ND2	ASN B 364	-23.102	59.746	22.325	1.00	55.95	7
	ATOM	782	C	ASN B 364	-25.494	63.771	22.091	1.00	31.89	6
	ATOM	783	O	ASN B 364	-26.279	63.471	22.990	1.00	30.28	8
	ATOM	784	N	LEU B 365	-25.306	65.018	21.673	1.00	27.62	7
50	ATOM	785	CA	LEU B 365	-26.005	66.144	22.280	1.00	29.36	6
	ATOM	786	CB	LEU B 365	-25.402	67.443	21.743	1.00	27.54	6
	ATOM	787	CG	LEU B 365	-23.897	67.453	21.738	1.00	38.91	6
	ATOM	788	CD1	LEU B 365	-23.391	68.766	21.190	1.00	34.47	6
55	ATOM	789	CD2	LEU B 365	-23.393	67.214	23.143	1.00	34.24	6
	ATOM	790	C	LEU B 365	-27.496	66.074	21.987	1.00	26.23	6
	ATOM	791	O	LEU B 365	-27.911	65.790	20.863	1.00	27.06	8
	ATOM	792	N	ASP B 366	-28.296	66.321	23.022	1.00	25.23	7
60	ATOM	793	CA	ASP B 366	-29.752	66.320	22.878	1.00	26.07	6
	ATOM	794	CB	ASP B 366	-30.441	65.651	24.076	1.00	29.68	6
	ATOM	795	CG	ASP B 366	-30.221	66.374	25.360	1.00	35.74	6
	ATOM	796	OD1	ASP B 366	-30.277	67.617	25.387	1.00	36.78	8
65	ATOM	797	OD2	ASP B 366	-30.017	65.711	26.410	1.00	41.23	8
	ATOM	798	C	ASP B 366	-30.230	67.752	22.740	1.00	27.70	6
	ATOM	799	O	ASP B 366	-29.552	68.678	23.171	1.00	31.94	8
	ATOM	800	N	ASP B 367	-31.409	67.913	22.142	1.00	29.18	7
70	ATOM	801	CA	ASP B 367	-32.031	69.225	21.930	1.00	32.72	6
	ATOM	802	CB	ASP B 367	-33.558	69.106	22.071	1.00	38.04	6

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5	ATOM	803	CG	ASP	B	367	-34.172	68.166	21.081	1.00	42.43	6
	ATOM	804	OD1	ASP	B	367	-34.051	68.373	19.854	1.00	35.95	8
	ATOM	805	OD2	ASP	B	367	-34.829	67.188	21.504	1.00	51.42	8
	ATOM	806	C	ASP	B	367	-31.496	70.238	22.959	1.00	33.71	6
	ATOM	807	O	ASP	B	367	-30.791	71.188	22.624	1.00	38.30	8
10	ATOM	808	N	THR	B	368	-31.858	69.997	24.218	1.00	31.06	7
	ATOM	809	CA	THR	B	368	-31.453	70.822	25.344	1.00	26.28	6
	ATOM	810	CB	THR	B	368	-31.567	70.020	26.643	1.00	27.30	6
	ATOM	811	OG1	THR	B	368	-32.916	69.578	26.824	1.00	33.42	8
	ATOM	812	CG2	THR	B	368	-31.143	70.855	27.824	1.00	25.16	6
15	ATOM	813	C	THR	B	368	-30.025	71.315	25.181	1.00	21.13	6
	ATOM	814	O	THR	B	368	-29.746	72.508	25.150	1.00	23.17	8
	ATOM	815	N	GLU	B	369	-29.123	70.354	25.072	1.00	21.32	7
	ATOM	816	CA	GLU	B	369	-27.711	70.634	24.932	1.00	28.00	6
	ATOM	817	CB	GLU	B	369	-26.947	69.306	24.878	1.00	32.79	6
20	ATOM	818	CG	GLU	B	369	-27.229	68.433	26.130	1.00	36.29	6
	ATOM	819	CD	GLU	B	369	-26.689	67.051	26.083	1.00	41.03	6
	ATOM	820	OE1	GLU	B	369	-26.960	66.318	25.102	1.00	42.05	8
	ATOM	821	OE2	GLU	B	369	-25.992	66.645	27.048	1.00	42.03	8
	ATOM	822	C	GLU	B	369	-27.428	71.527	23.731	1.00	25.57	6
25	ATOM	823	O	GLU	B	369	-26.780	72.549	23.886	1.00	20.56	8
	ATOM	824	N	VAL	B	370	-27.922	71.154	22.548	1.00	25.39	7
	ATOM	825	CA	VAL	B	370	-27.710	71.968	21.355	1.00	25.99	6
	ATOM	826	CB	VAL	B	370	-28.457	71.429	20.130	1.00	26.15	6
	ATOM	827	CG1	VAL	B	370	-28.255	72.358	18.953	1.00	27.65	6
30	ATOM	828	CG2	VAL	B	370	-28.014	70.021	19.788	1.00	17.70	6
	ATOM	829	C	VAL	B	370	-28.238	73.346	21.676	1.00	26.49	6
	ATOM	830	O	VAL	B	370	-27.580	74.351	21.445	1.00	28.16	8
	ATOM	831	N	ALA	B	371	-29.450	73.362	22.213	1.00	21.01	7
	ATOM	832	CA	ALA	B	371	-30.145	74.589	22.573	1.00	19.57	6
35	ATOM	833	CB	ALA	B	371	-31.414	74.246	23.335	1.00	18.62	6
	ATOM	834	C	ALA	B	371	-29.256	75.501	23.401	1.00	23.48	6
	ATOM	835	O	ALA	B	371	-28.936	76.613	22.989	1.00	32.67	8
	ATOM	836	N	LEU	B	372	-28.860	75.008	24.571	1.00	22.89	7
	ATOM	837	CA	LEU	B	372	-27.999	75.758	25.472	1.00	23.28	6
40	ATOM	838	CB	LEU	B	372	-27.606	74.860	26.658	1.00	27.76	6
	ATOM	839	CG	LEU	B	372	-28.728	74.524	27.619	1.00	21.18	6
	ATOM	840	CD1	LEU	B	372	-28.272	73.529	28.648	1.00	27.64	6
	ATOM	841	CD2	LEU	B	372	-29.198	75.801	28.284	1.00	20.90	6
	ATOM	842	C	LEU	B	372	-26.769	76.268	24.722	1.00	21.34	6
45	ATOM	843	O	LEU	B	372	-26.439	77.454	24.762	1.00	23.16	8
	ATOM	844	N	LEU	B	373	-26.111	75.349	24.023	1.00	24.42	7
	ATOM	845	CA	LEU	B	373	-24.916	75.669	23.254	1.00	23.78	6
	ATOM	846	CB	LEU	B	373	-24.525	74.446	22.396	1.00	22.18	6
	ATOM	847	CG	LEU	B	373	-23.098	74.283	21.942	1.00	31.52	6
50	ATOM	848	CD1	LEU	B	373	-22.196	74.576	23.100	1.00	31.93	6
	ATOM	849	CD2	LEU	B	373	-22.873	72.889	21.457	1.00	30.24	6
	ATOM	850	C	LEU	B	373	-25.235	76.902	22.405	1.00	25.69	6
	ATOM	851	O	LEU	B	373	-24.491	77.880	22.416	1.00	30.13	8
	ATOM	852	N	GLN	B	374	-26.368	76.842	21.707	1.00	26.24	7
55	ATOM	853	CA	GLN	B	374	-26.836	77.922	20.839	1.00	21.60	6
	ATOM	854	CB	GLN	B	374	-28.196	77.571	20.221	1.00	24.57	6
	ATOM	855	CG	GLN	B	374	-28.188	76.330	19.348	1.00	21.02	6
	ATOM	856	CD	GLN	B	374	-29.538	76.071	18.698	1.00	22.86	6

5	ATOM	857	OE1	GLN B 374	-29.720	75.049	18.009	1.00	24.07	8
	ATOM	858	NE2	GLN B 374	-30.473	76.980	18.901	1.00	25.59	7
	ATOM	859	C	GLN B 374	-26.988	79.249	21.569	1.00	20.66	6
	ATOM	860	O	GLN B 374	-26.733	80.307	20.994	1.00	24.47	8
10	ATOM	861	N	ALA B 375	-27.429	79.182	22.825	1.00	16.26	7
	ATOM	862	CA	ALA B 375	-27.639	80.374	23.631	1.00	17.16	6
	ATOM	863	CB	ALA B 375	-28.435	80.025	24.865	1.00	19.53	6
	ATOM	864	C	ALA B 375	-26.304	80.966	24.025	1.00	25.13	6
15	ATOM	865	O	ALA B 375	-26.074	82.154	23.833	1.00	23.81	8
	ATOM	866	N	VAL B 376	-25.433	80.111	24.568	1.00	24.57	7
	ATOM	867	CA	VAL B 376	-24.102	80.526	24.986	1.00	25.80	6
	ATOM	868	CB	VAL B 376	-23.192	79.321	25.234	1.00	26.48	6
20	ATOM	869	CG1	VAL B 376	-21.806	79.780	25.620	1.00	23.20	6
	ATOM	870	CG2	VAL B 376	-23.771	78.433	26.310	1.00	19.08	6
	ATOM	871	C	VAL B 376	-23.510	81.403	23.898	1.00	25.69	6
	ATOM	872	O	VAL B 376	-22.796	82.364	24.166	1.00	27.87	8
25	ATOM	873	N	LEU B 377	-23.827	81.049	22.659	1.00	23.09	7
	ATOM	874	CA	LEU B 377	-23.340	81.774	21.492	1.00	22.86	6
	ATOM	875	CB	LEU B 377	-23.552	80.920	20.230	1.00	18.50	6
	ATOM	876	CG	LEU B 377	-22.756	79.638	20.146	1.00	22.65	6
30	ATOM	877	CD1	LEU B 377	-23.221	78.786	19.000	1.00	16.70	6
	ATOM	878	CD2	LEU B 377	-21.300	79.995	20.000	1.00	19.58	6
	ATOM	879	C	LEU B 377	-24.073	83.102	21.384	1.00	26.14	6
	ATOM	880	O	LEU B 377	-23.464	84.164	21.419	1.00	20.62	8
35	ATOM	881	N	LEU B 378	-25.396	83.023	21.265	1.00	28.99	7
	ATOM	882	CA	LEU B 378	-26.228	84.217	21.147	1.00	28.87	6
	ATOM	883	CB	LEU B 378	-27.696	83.894	21.450	1.00	26.89	6
	ATOM	884	CG	LEU B 378	-28.648	85.068	21.500	1.00	28.83	6
40	ATOM	885	CD1	LEU B 378	-28.507	85.854	20.225	1.00	27.97	6
	ATOM	886	CD2	LEU B 378	-30.072	84.605	21.692	1.00	27.69	6
	ATOM	887	C	LEU B 378	-25.738	85.280	22.090	1.00	31.09	6
	ATOM	888	O	LEU B 378	-25.398	86.379	21.651	1.00	31.77	8
45	ATOM	889	N	MET B 379	-25.695	84.931	23.376	1.00	31.44	7
	ATOM	890	CA	MET B 379	-25.291	85.851	24.434	1.00	32.62	6
	ATOM	891	CB	MET B 379	-25.797	85.335	25.793	1.00	31.45	6
	ATOM	892	CG	MET B 379	-27.332	85.262	25.883	1.00	38.75	6
50	ATOM	893	SD	MET B 379	-28.020	86.915	25.550	1.00	41.27	16
	ATOM	894	CE	MET B 379	-29.814	86.586	25.513	1.00	35.68	6
	ATOM	895	C	MET B 379	-23.796	86.129	24.538	1.00	33.72	6
	ATOM	896	O	MET B 379	-23.246	86.190	25.633	1.00	36.29	8
55	ATOM	897	N	SER B 380	-23.152	86.335	23.399	1.00	34.49	7
	ATOM	898	CA	SER B 380	-21.738	86.659	23.391	1.00	33.97	6
	ATOM	899	CB	SER B 380	-21.132	86.360	22.010	1.00	31.24	6
	ATOM	900	OG	SER B 380	-21.224	84.978	21.696	1.00	39.42	8
60	ATOM	901	C	SER B 380	-21.635	88.145	23.705	1.00	39.69	6
	ATOM	902	O	SER B 380	-22.084	88.989	22.933	1.00	44.64	8
	ATOM	903	N	SER B 381	-21.053	88.451	24.857	1.00	41.04	7
	ATOM	904	CA	SER B 381	-20.907	89.826	25.308	1.00	44.91	6
65	ATOM	905	CB	SER B 381	-20.610	89.832	26.797	1.00	44.50	6
	ATOM	906	OG	SER B 381	-19.351	89.229	27.037	1.00	45.42	8
	ATOM	907	C	SER B 381	-19.815	90.614	24.602	1.00	44.59	6
	ATOM	908	O	SER B 381	-19.725	91.825	24.751	1.00	49.32	8
70	ATOM	909	N	ASP B 382	-18.977	89.922	23.848	1.00	43.75	7
	ATOM	910	CA	ASP B 382	-17.886	90.556	23.144	1.00	43.93	6

5	ATOM	911	CB	ASP	B	382	-16.727	89.562	23.028	1.00	48.39	6
	ATOM	912	CG	ASP	B	382	-17.142	88.232	22.471	1.00	53.23	6
	ATOM	913	OD1	ASP	B	382	-18.102	87.621	23.002	1.00	56.97	8
	ATOM	914	OD2	ASP	B	382	-16.513	87.753	21.480	1.00	58.91	8
	ATOM	915	C	ASP	B	382	-18.191	91.172	21.772	1.00	41.09	6
10	ATOM	916	O	ASP	B	382	-17.366	91.899	21.229	1.00	40.93	8
	ATOM	917	N	ARG	B	383	-19.369	90.908	21.224	1.00	42.63	7
	ATOM	918	CA	ARG	B	383	-19.698	91.445	19.934	1.00	43.32	6
	ATOM	919	CB	ARG	B	383	-21.131	91.101	19.557	1.00	42.31	6
	ATOM	920	CG	ARG	B	383	-21.619	89.672	19.811	1.00	40.83	6
15	ATOM	921	CD	ARG	B	383	-21.144	88.627	18.804	1.00	38.09	6
	ATOM	922	NE	ARG	B	383	-21.922	87.415	18.943	1.00	37.33	7
	ATOM	923	CZ	ARG	B	383	-21.584	86.250	18.411	1.00	38.35	6
	ATOM	924	NH1	ARG	B	383	-20.465	86.143	17.700	1.00	33.70	7
	ATOM	925	NH2	ARG	B	383	-22.369	85.196	18.604	1.00	35.46	7
20	ATOM	926	C	ARG	B	383	-19.591	92.958	20.007	1.00	44.96	6
	ATOM	927	O	ARG	B	383	-20.050	93.577	20.980	1.00	45.60	8
	ATOM	928	N	PRO	B	384	-18.975	93.579	19.005	1.00	45.33	7
	ATOM	929	CD	PRO	B	384	-18.395	92.881	17.854	1.00	46.85	6
	ATOM	930	CA	PRO	B	384	-18.808	95.035	18.947	1.00	47.37	6
25	ATOM	931	CB	PRO	B	384	-17.868	95.255	17.764	1.00	46.90	6
	ATOM	932	CG	PRO	B	384	-17.575	93.934	17.187	1.00	46.41	6
	ATOM	933	C	PRO	B	384	-20.125	95.778	18.762	1.00	48.29	6
	ATOM	934	O	PRO	B	384	-21.048	95.277	18.120	1.00	48.34	8
	ATOM	935	N	GLY	B	385	-20.185	96.994	19.314	1.00	49.88	7
30	ATOM	936	CA	GLY	B	385	-21.371	97.838	19.192	1.00	50.35	6
	ATOM	937	C	GLY	B	385	-22.410	97.615	20.265	1.00	50.70	6
	ATOM	938	O	GLY	B	385	-23.382	98.363	20.374	1.00	53.48	8
	ATOM	939	N	LEU	B	386	-22.205	96.557	21.044	1.00	49.04	7
	ATOM	940	CA	LEU	B	386	-23.136	96.211	22.101	1.00	50.53	6
35	ATOM	941	CB	LEU	B	386	-22.640	94.972	22.853	1.00	45.17	6
	ATOM	942	CG	LEU	B	386	-22.744	93.653	22.121	1.00	48.26	6
	ATOM	943	CD1	LEU	B	386	-22.122	92.525	22.938	1.00	41.68	6
	ATOM	944	CD2	LEU	B	386	-24.215	93.376	21.852	1.00	38.40	6
	ATOM	945	C	LEU	B	386	-23.322	97.357	23.058	1.00	52.13	6
40	ATOM	946	O	LEU	B	386	-22.438	98.182	23.234	1.00	53.67	8
	ATOM	947	N	ALA	B	387	-24.499	97.398	23.666	1.00	53.42	7
	ATOM	948	CA	ALA	B	387	-24.830	98.441	24.624	1.00	56.01	6
	ATOM	949	CB	ALA	B	387	-26.223	98.993	24.339	1.00	56.47	6
	ATOM	950	C	ALA	B	387	-24.775	97.853	26.024	1.00	55.52	6
45	ATOM	951	O	ALA	B	387	-23.798	98.027	26.753	1.00	53.75	8
	ATOM	952	N	CYS	B	388	-25.843	97.145	26.371	1.00	56.03	7
	ATOM	953	CA	CYS	B	388	-26.000	96.525	27.673	1.00	59.57	6
	ATOM	954	CB	CYS	B	388	-27.469	96.134	27.839	1.00	59.23	6
	ATOM	955	SG	CYS	B	388	-28.620	97.392	27.264	1.00	58.64	16
50	ATOM	956	C	CYS	B	388	-25.105	95.283	27.798	1.00	62.18	6
	ATOM	957	O	CYS	B	388	-25.590	94.164	27.868	1.00	67.88	8
	ATOM	958	N	VAL	B	389	-23.789	95.510	27.824	1.00	60.78	7
	ATOM	959	CA	VAL	B	389	-22.797	94.434	27.959	1.00	57.70	6
	ATOM	960	CB	VAL	B	389	-21.355	94.976	27.998	1.00	57.09	6
55	ATOM	961	CG1	VAL	B	389	-20.361	93.832	28.085	1.00	59.03	6
	ATOM	962	CG2	VAL	B	389	-21.065	95.845	26.791	1.00	53.98	6
	ATOM	963	C	VAL	B	389	-23.078	93.642	29.230	1.00	57.77	6
	ATOM	964	O	VAL	B	389	-23.727	92.602	29.203	1.00	60.94	8

					-22.561	94.159	30.332	1.00	52.68	7
5	ATOM	965	N	ALA B 390	-22.684	93.570	31.659	1.00	48.41	6
	ATOM	966	CA	ALA B 390	-22.650	94.681	32.716	1.00	45.19	6
	ATOM	967	CB	ALA B 390	-23.905	92.697	31.877	1.00	47.63	6
	ATOM	968	C	ALA B 390	-23.784	91.576	32.369	1.00	51.95	8
	ATOM	969	O	ALA B 390	-25.075	93.216	31.498	1.00	47.11	7
10	ATOM	970	N	ARG B 391	-26.330	92.481	31.656	1.00	51.64	6
	ATOM	971	CA	ARG B 391	-27.502	93.318	31.122	1.00	54.22	6
	ATOM	972	CB	ARG B 391	-28.887	92.713	31.430	1.00	64.20	6
	ATOM	973	CG	ARG B 391	-30.059	93.582	30.929	1.00	73.80	6
	ATOM	974	CD	ARG B 391	-31.361	93.097	31.378	1.00	79.76	7
15	ATOM	975	NE	ARG B 391	-31.736	93.015	32.656	1.00	84.27	6
	ATOM	976	CZ	ARG B 391	-30.887	93.372	33.625	1.00	85.28	7
	ATOM	977	NH1	ARG B 391	-32.957	92.566	32.955	1.00	86.84	7
	ATOM	978	NH2	ARG B 391	-26.277	91.133	30.940	1.00	48.18	6
	ATOM	979	C	ARG B 391	-26.724	90.119	31.465	1.00	49.57	8
20	ATOM	980	O	ARG B 391	-25.743	91.167	29.718	1.00	45.01	7
	ATOM	981	N	ILE B 392	-25.592	89.999	28.867	1.00	48.77	6
	ATOM	982	CA	ILE B 392	-25.112	90.424	27.469	1.00	46.45	6
	ATOM	983	CB	ILE B 392	-24.805	89.221	26.614	1.00	42.35	6
	ATOM	984	CG2	ILE B 392	-26.178	91.283	26.768	1.00	49.69	6
25	ATOM	985	CG1	ILE B 392	-25.762	91.768	25.386	1.00	51.09	6
	ATOM	986	CD1	ILE B 392	-24.671	88.935	29.462	1.00	50.90	6
	ATOM	987	C	ILE B 392	-25.086	87.780	29.605	1.00	52.21	8
	ATOM	988	O	ILE B 392	-23.431	89.298	29.790	1.00	50.43	7
	ATOM	989	N	GLU B 393	-22.504	88.328	30.378	1.00	50.30	6
30	ATOM	990	CA	GLU B 393	-21.314	89.022	31.044	1.00	53.97	6
	ATOM	991	CB	GLU B 393	-20.063	89.005	30.209	1.00	62.18	6
	ATOM	992	CG	GLU B 393	-18.877	89.415	30.976	1.00	67.69	6
	ATOM	993	CD	GLU B 393	-17.709	89.264	30.656	1.00	66.42	8
	ATOM	994	OE1	GLU B 393	-18.897	89.976	32.052	1.00	70.64	8
35	ATOM	995	OE2	GLU B 393	-23.251	87.477	31.416	1.00	49.31	6
	ATOM	996	C	GLU B 393	-23.226	86.260	31.303	1.00	49.53	8
	ATOM	997	O	GLU B 393	-23.898	88.153	32.409	1.00	46.07	7
	ATOM	998	N	LYS B 394	-24.721	87.579	33.506	1.00	45.76	6
	ATOM	999	CA	LYS B 394	-25.594	88.693	34.161	1.00	43.85	6
40	ATOM	1000	CB	LYS B 394	-25.626	86.548	32.851	1.00	46.69	6
	ATOM	1001	C	LYS B 394	-25.772	85.430	33.329	1.00	49.13	8
	ATOM	1002	O	LYS B 394	-26.203	86.948	31.719	1.00	46.57	7
	ATOM	1003	N	TYR B 395	-27.076	86.078	30.938	1.00	43.33	6
	ATOM	1004	CA	TYR B 395	-27.621	86.821	29.716	1.00	48.44	6
45	ATOM	1005	CB	TYR B 395	-28.827	87.688	29.980	1.00	53.83	6
	ATOM	1006	CG	TYR B 395	-29.204	88.680	29.080	1.00	56.43	6
	ATOM	1007	CD1	TYR B 395	-30.331	89.469	29.309	1.00	59.73	6
	ATOM	1008	CE1	TYR B 395	-29.596	87.509	31.113	1.00	56.47	6
	ATOM	1009	CD2	TYR B 395	-30.723	88.295	31.346	1.00	62.60	6
50	ATOM	1010	CE2	TYR B 395	-31.090	89.281	30.446	1.00	63.18	6
	ATOM	1011	CZ	TYR B 395	-32.189	90.068	30.671	1.00	64.46	8
	ATOM	1012	OH	TYR B 395	-26.276	84.867	30.485	1.00	37.30	6
	ATOM	1013	C	TYR B 395	-26.611	83.737	30.825	1.00	34.10	8
	ATOM	1014	O	TYR B 395	-25.213	85.108	29.718	1.00	31.92	7
55	ATOM	1015	N	GLN B 396	-24.380	84.018	29.244	1.00	34.81	6
	ATOM	1016	CA	GLN B 396	-23.176	84.550	28.464	1.00	32.64	6
	ATOM	1017	CB	GLN B 396	-22.184	83.470	28.103	1.00	29.57	6
	ATOM	1018	CG	GLN B 396						



5	ATOM	1019	CD	GLN	B	396	-21.214	83.871	27.016	1.00	29.46	6
	ATOM	1020	OE1	GLN	B	396	-20.547	84.930	27.109	1.00	34.65	8
	ATOM	1021	NE2	GLN	B	396	-21.112	83.032	25.992	1.00	27.21	7
	ATOM	1022	C	GLN	B	396	-23.908	83.207	30.434	1.00	37.13	6
10	ATOM	1023	O	GLN	B	396	-23.876	81.986	30.384	1.00	37.36	8
	ATOM	1024	N	ASP	B	397	-23.544	83.903	31.508	1.00	38.61	7
	ATOM	1025	CA	ASP	B	397	-23.069	83.250	32.717	1.00	40.37	6
	ATOM	1026	CB	ASP	B	397	-22.617	84.297	33.754	1.00	40.51	6
15	ATOM	1027	CG	ASP	B	397	-21.360	85.025	33.352	1.00	43.77	6
	ATOM	1028	OD1	ASP	B	397	-20.337	84.366	33.054	1.00	46.50	8
	ATOM	1029	OD2	ASP	B	397	-21.343	86.287	33.350	1.00	51.34	8
	ATOM	1030	C	ASP	B	397	-24.223	82.422	33.267	1.00	38.62	6
20	ATOM	1031	O	ASP	B	397	-24.023	81.327	33.778	1.00	39.20	8
	ATOM	1032	N	SER	B	398	-25.432	82.962	33.138	1.00	37.84	7
	ATOM	1033	CA	SER	B	398	-26.633	82.293	33.622	1.00	37.80	6
	ATOM	1034	CB	SER	B	398	-27.830	83.246	33.501	1.00	34.28	6
25	ATOM	1035	OG	SER	B	398	-28.995	82.715	34.114	1.00	46.60	8
	ATOM	1036	C	SER	B	398	-26.911	80.997	32.867	1.00	38.41	6
	ATOM	1037	O	SER	B	398	-27.454	80.047	33.433	1.00	39.98	8
	ATOM	1038	N	PHE	B	399	-26.546	80.963	31.587	1.00	34.82	7
30	ATOM	1039	CA	PHE	B	399	-26.772	79.768	30.781	1.00	35.96	6
	ATOM	1040	CB	PHE	B	399	-26.892	80.100	29.293	1.00	35.75	6
	ATOM	1041	CG	PHE	B	399	-28.211	80.717	28.906	1.00	39.30	6
	ATOM	1042	CD1	PHE	B	399	-28.466	82.056	29.109	1.00	39.86	6
35	ATOM	1043	CD2	PHE	B	399	-29.194	79.938	28.355	1.00	36.81	6
	ATOM	1044	CE1	PHE	B	399	-29.700	82.602	28.739	1.00	41.25	6
	ATOM	1045	CE2	PHE	B	399	-30.424	80.483	27.987	1.00	43.61	6
	ATOM	1046	CZ	PHE	B	399	-30.677	81.813	28.181	1.00	40.34	6
40	ATOM	1047	C	PHE	B	399	-25.658	78.754	30.976	1.00	33.48	6
	ATOM	1048	O	PHE	B	399	-25.927	77.589	31.256	1.00	26.86	8
	ATOM	1049	N	LEU	B	400	-24.408	79.187	30.796	1.00	31.47	7
	ATOM	1050	CA	LEU	B	400	-23.275	78.291	30.945	1.00	37.41	6
45	ATOM	1051	CB	LEU	B	400	-21.976	79.091	31.030	1.00	34.24	6
	ATOM	1052	CG	LEU	B	400	-21.470	79.642	29.726	1.00	35.10	6
	ATOM	1053	CD1	LEU	B	400	-20.121	80.304	29.917	1.00	26.60	6
	ATOM	1054	CD2	LEU	B	400	-21.326	78.488	28.759	1.00	29.44	6
50	ATOM	1055	C	LEU	B	400	-23.430	77.376	32.145	1.00	38.84	6
	ATOM	1056	O	LEU	B	400	-23.366	76.157	32.007	1.00	40.38	8
	ATOM	1057	N	LEU	B	401	-23.639	77.968	33.321	1.00	42.79	7
	ATOM	1058	CA	LEU	B	401	-23.801	77.181	34.537	1.00	43.48	6
55	ATOM	1059	CB	LEU	B	401	-24.226	78.067	35.712	1.00	44.73	6
	ATOM	1060	CG	LEU	B	401	-24.378	77.303	37.012	1.00	51.39	6
	ATOM	1061	CD1	LEU	B	401	-22.990	76.844	37.484	1.00	50.11	6
	ATOM	1062	CD2	LEU	B	401	-25.027	78.163	38.083	1.00	49.30	6
60	ATOM	1063	C	LEU	B	401	-24.854	76.095	34.311	1.00	41.62	6
	ATOM	1064	O	LEU	B	401	-24.576	74.900	34.427	1.00	45.14	8
	ATOM	1065	N	ALA	B	402	-26.068	76.532	33.997	1.00	37.92	7
	ATOM	1066	CA	ALA	B	402	-27.177	75.631	33.752	1.00	29.90	6
65	ATOM	1067	CB	ALA	B	402	-28.361	76.433	33.200	1.00	30.70	6
	ATOM	1068	C	ALA	B	402	-26.779	74.521	32.773	1.00	28.88	6
	ATOM	1069	O	ALA	B	402	-27.078	73.347	32.996	1.00	32.14	8
	ATOM	1070	N	PHE	B	403	-26.091	74.908	31.698	1.00	31.07	7
70	ATOM	1071	CA	PHE	B	403	-25.655	73.970	30.673	1.00	29.90	6
	ATOM	1072	CB	PHE	B	403	-24.847	74.715	29.607	1.00	27.03	6

5	ATOM	1073	CG	PHE B 403	-24.557	73.904	27.272	1.00	25.55	6
	ATOM	1074	CD1	PHE B 403	-23.916	74.494	27.272	1.00	25.55	6
	ATOM	1075	CD2	PHE B 403	-24.939	72.583	28.271	1.00	19.75	6
	ATOM	1076	CE1	PHE B 403	-23.670	73.765	26.104	1.00	27.90	6
	ATOM	1077	CE2	PHE B 403	-24.693	71.848	27.102	1.00	22.56	6
10	ATOM	1078	CZ	PHE B 403	-24.057	72.439	26.020	1.00	22.24	6
	ATOM	1079	C	PHE B 403	-24.810	72.902	31.329	1.00	28.82	6
	ATOM	1080	O	PHE B 403	-25.092	71.726	31.205	1.00	26.00	8
	ATOM	1081	N	GLU B 404	-23.776	73.335	32.037	1.00	30.25	7
15	ATOM	1082	CA	GLU B 404	-22.865	72.419	32.712	1.00	34.03	6
	ATOM	1083	CB	GLU B 404	-21.835	73.215	33.527	1.00	39.45	6
	ATOM	1084	CG	GLU B 404	-20.654	72.384	34.068	1.00	47.68	6
	ATOM	1085	CD	GLU B 404	-19.750	73.129	34.996	1.00	54.02	6
	ATOM	1086	OE1	GLU B 404	-19.372	74.290	34.701	1.00	57.27	8
20	ATOM	1087	OE2	GLU B 404	-19.369	72.555	36.048	1.00	63.85	8
	ATOM	1088	C	GLU B 404	-23.645	71.509	33.642	1.00	36.01	6
	ATOM	1089	O	GLU B 404	-23.470	70.292	33.640	1.00	38.64	8
	ATOM	1090	N	HIS B 405	-24.492	72.131	34.458	1.00	29.56	7
	ATOM	1091	CA	HIS B 405	-25.306	71.387	35.405	1.00	31.69	6
25	ATOM	1092	CB	HIS B 405	-26.245	72.324	36.173	1.00	33.75	6
	ATOM	1093	CG	HIS B 405	-25.536	73.185	37.163	1.00	34.75	6
	ATOM	1094	CD2	HIS B 405	-24.234	73.286	37.524	1.00	34.58	6
	ATOM	1095	ND1	HIS B 405	-26.223	74.101	37.969	1.00	32.43	7
	ATOM	1096	CE1	HIS B 405	-25.334	74.703	38.769	1.00	36.15	6
30	ATOM	1097	NE2	HIS B 405	-24.139	74.222	38.511	1.00	39.84	7
	ATOM	1098	C	HIS B 405	-26.106	70.342	34.648	1.00	34.21	6
	ATOM	1099	O	HIS B 405	-26.087	69.160	35.006	1.00	37.06	8
	ATOM	1100	N	TYR B 406	-26.806	70.776	33.598	1.00	30.83	7
	ATOM	1101	CA	TYR B 406	-27.592	69.853	32.796	1.00	28.85	6
35	ATOM	1102	CB	TYR B 406	-28.192	70.537	31.579	1.00	31.48	6
	ATOM	1103	CG	TYR B 406	-28.991	69.576	30.730	1.00	23.49	6
	ATOM	1104	CD1	TYR B 406	-30.179	69.047	31.196	1.00	19.42	6
	ATOM	1105	CE1	TYR B 406	-30.893	68.128	30.441	1.00	23.80	6
	ATOM	1106	CD2	TYR B 406	-28.525	69.152	29.496	1.00	21.81	6
40	ATOM	1107	CE2	TYR B 406	-29.241	68.228	28.740	1.00	24.64	6
	ATOM	1108	CZ	TYR B 406	-30.420	67.713	29.217	1.00	21.56	6
	ATOM	1109	OH	TYR B 406	-31.120	66.802	28.480	1.00	24.96	8
	ATOM	1110	C	TYR B 406	-26.697	68.725	32.304	1.00	24.24	6
	ATOM	1111	O	TYR B 406	-27.155	67.609	32.110	1.00	27.08	8
45	ATOM	1112	N	ILE B 407	-25.422	69.056	32.084	1.00	25.76	7
	ATOM	1113	CA	ILE B 407	-24.428	68.092	31.628	1.00	33.75	6
	ATOM	1114	CB	ILE B 407	-23.090	68.778	31.274	1.00	34.23	6
	ATOM	1115	CG2	ILE B 407	-21.959	67.774	31.230	1.00	32.46	6
	ATOM	1116	CG1	ILE B 407	-23.214	69.514	29.936	1.00	43.30	6
50	ATOM	1117	CD1	ILE B 407	-23.655	68.612	28.804	1.00	40.40	6
	ATOM	1118	C	ILE B 407	-24.191	67.004	32.658	1.00	39.03	6
	ATOM	1119	O	ILE B 407	-24.178	65.806	32.343	1.00	35.18	8
	ATOM	1120	N	ASN B 408	-23.990	67.425	33.894	1.00	37.25	7
	ATOM	1121	CA	ASN B 408	-23.739	66.475	34.943	1.00	37.01	6
55	ATOM	1122	CB	ASN B 408	-23.524	67.221	36.256	1.00	32.27	6
	ATOM	1123	CG	ASN B 408	-22.296	68.137	36.202	1.00	33.56	6
	ATOM	1124	OD1	ASN B 408	-21.194	67.696	35.823	1.00	31.99	8
	ATOM	1125	ND2	ASN B 408	-22.478	69.397	36.604	1.00	31.23	7
	ATOM	1126	C	ASN B 408	-24.876	65.453	35.036	1.00	38.14	6

5	ATOM	1127	O	ASN	B	408	-24.624	64.253	35.105	1.00	42.16	8
	ATOM	1128	N	TYR	B	409	-26.122	65.924	35.003	1.00	35.62	7
	ATOM	1129	CA	TYR	B	409	-27.273	65.024	35.073	1.00	35.91	6
	ATOM	1130	CB	TYR	B	409	-28.597	65.787	34.931	1.00	34.41	6
	ATOM	1131	CG	TYR	B	409	-29.788	64.868	34.685	1.00	38.73	6
10	ATOM	1132	CD1	TYR	B	409	-30.064	63.819	35.549	1.00	41.34	6
	ATOM	1133	CE1	TYR	B	409	-31.130	62.962	35.309	1.00	47.16	6
	ATOM	1134	CD2	TYR	B	409	-30.613	65.037	33.579	1.00	46.20	6
	ATOM	1135	CE2	TYR	B	409	-31.684	64.176	33.341	1.00	50.74	6
	ATOM	1136	CZ	TYR	B	409	-31.942	63.143	34.206	1.00	50.88	6
15	ATOM	1137	OH	TYR	B	409	-33.002	62.312	33.978	1.00	53.14	8
	ATOM	1138	C	TYR	B	409	-27.215	64.020	33.951	1.00	38.16	6
	ATOM	1139	O	TYR	B	409	-27.558	62.857	34.111	1.00	41.83	8
	ATOM	1140	N	ARG	B	410	-26.824	64.528	32.796	1.00	42.25	7
	ATOM	1141	CA	ARG	B	410	-26.734	63.739	31.594	1.00	42.83	6
20	ATOM	1142	CB	ARG	B	410	-26.350	64.646	30.441	1.00	36.83	6
	ATOM	1143	CG	ARG	B	410	-27.440	65.585	29.945	1.00	34.32	6
	ATOM	1144	CD	ARG	B	410	-28.284	64.863	28.917	1.00	36.62	6
	ATOM	1145	NE	ARG	B	410	-27.455	64.378	27.829	1.00	38.64	7
	ATOM	1146	CZ	ARG	B	410	-27.926	63.656	26.824	1.00	35.73	6
25	ATOM	1147	NH1	ARG	B	410	-29.234	63.379	26.782	1.00	33.17	7
	ATOM	1148	NH2	ARG	B	410	-27.095	63.227	25.868	1.00	32.70	7
	ATOM	1149	C	ARG	B	410	-25.688	62.664	31.733	1.00	46.67	6
	ATOM	1150	O	ARG	B	410	-25.859	61.547	31.257	1.00	41.78	8
	ATOM	1151	N	LYS	B	411	-24.602	63.028	32.413	1.00	52.99	7
30	ATOM	1152	CA	LYS	B	411	-23.471	62.145	32.609	1.00	58.32	6
	ATOM	1153	CB	LYS	B	411	-23.684	61.249	33.833	1.00	64.99	6
	ATOM	1154	CG	LYS	B	411	-24.998	60.544	33.968	1.00	70.48	6
	ATOM	1155	CD	LYS	B	411	-25.070	59.887	35.349	1.00	77.18	6
	ATOM	1156	CE	LYS	B	411	-26.272	58.944	35.474	1.00	84.30	6
35	ATOM	1157	NZ	LYS	B	411	-26.286	58.242	36.809	1.00	86.48	7
	ATOM	1158	C	LYS	B	411	-23.172	61.341	31.365	1.00	56.66	6
	ATOM	1159	O	LYS	B	411	-23.574	60.199	31.210	1.00	55.47	8
	ATOM	1160	N	HIS	B	412	-22.458	62.026	30.479	1.00	54.67	7
	ATOM	1161	CA	HIS	B	412	-22.019	61.474	29.214	1.00	48.67	6
40	ATOM	1162	CB	HIS	B	412	-21.500	62.599	28.310	1.00	43.14	6
	ATOM	1163	CG	HIS	B	412	-22.559	63.501	27.784	1.00	41.36	6
	ATOM	1164	CD2	HIS	B	412	-23.159	64.603	28.299	1.00	35.44	6
	ATOM	1165	ND1	HIS	B	412	-23.163	63.290	26.539	1.00	38.19	7
	ATOM	1166	CE1	HIS	B	412	-24.076	64.238	26.353	1.00	34.75	6
45	ATOM	1167	NE2	HIS	B	412	-24.090	65.034	27.396	1.00	35.52	7
	ATOM	1168	C	HIS	B	412	-20.894	60.596	29.644	1.00	46.35	6
	ATOM	1169	O	HIS	B	412	-20.218	60.892	30.644	1.00	42.73	8
	ATOM	1170	N	HIS	B	413	-20.708	59.469	28.973	1.00	48.92	7
	ATOM	1171	CA	HIS	B	413	-19.593	58.614	29.371	1.00	53.15	6
50	ATOM	1172	CB	HIS	B	413	-20.022	57.147	29.421	1.00	55.27	6
	ATOM	1173	CG	HIS	B	413	-20.814	56.823	30.636	1.00	58.77	6
	ATOM	1174	CD2	HIS	B	413	-22.019	56.223	30.822	1.00	61.65	6
	ATOM	1175	ND1	HIS	B	413	-20.360	57.159	31.921	1.00	60.31	7
	ATOM	1176	CE1	HIS	B	413	-21.267	56.758	32.809	1.00	63.01	6
55	ATOM	1177	NE2	HIS	B	413	-22.270	56.193	32.171	1.00	62.93	7
	ATOM	1178	C	HIS	B	413	-18.426	58.862	28.438	1.00	53.19	6
	ATOM	1179	O	HIS	B	413	-17.975	57.996	27.699	1.00	54.93	8
	ATOM	1180	N	VAL	B	414	-17.970	60.113	28.521	1.00	53.77	7

5	ATOM	1181	CA	VAL B 414	-16.845	60.674	27.788	1.00	51.06	6
	ATOM	1182	CB	VAL B 414	-17.317	61.498	26.586	1.00	51.49	6
	ATOM	1183	CG1	VAL B 414	-16.133	62.122	25.891	1.00	45.22	6
	ATOM	1184	CG2	VAL B 414	-18.095	60.631	25.617	1.00	52.67	6
	ATOM	1185	C	VAL B 414	-16.096	61.557	28.775	1.00	54.28	6
10	ATOM	1186	O	VAL B 414	-16.700	62.283	29.574	1.00	55.49	8
	ATOM	1187	N	THR B 415	-14.770	61.466	28.742	1.00	56.28	7
	ATOM	1188	CA	THR B 415	-13.919	62.234	29.669	1.00	57.83	6
	ATOM	1189	CB	THR B 415	-12.488	61.686	29.658	1.00	59.64	6
	ATOM	1190	OG1	THR B 415	-11.618	62.572	30.373	1.00	66.69	8
15	ATOM	1191	CG2	THR B 415	-11.988	61.483	28.227	1.00	59.42	6
	ATOM	1192	C	THR B 415	-13.840	63.726	29.352	1.00	56.98	6
	ATOM	1193	O	THR B 415	-13.987	64.135	28.216	1.00	55.70	8
	ATOM	1194	N	HIS B 416	-13.598	64.522	30.387	1.00	57.44	7
	ATOM	1195	CA	HIS B 416	-13.485	65.972	30.237	1.00	57.34	6
20	ATOM	1196	CB	HIS B 416	-12.114	66.326	29.653	1.00	61.35	6
	ATOM	1197	CG	HIS B 416	-10.968	65.931	30.513	1.00	69.78	6
	ATOM	1198	CD2	HIS B 416	-9.930	65.082	30.307	1.00	71.42	6
	ATOM	1199	ND1	HIS B 416	-10.756	66.480	31.787	1.00	72.49	7
	ATOM	1200	CE1	HIS B 416	-9.631	65.973	32.281	1.00	75.50	6
25	ATOM	1201	NE2	HIS B 416	-9.120	65.131	31.408	1.00	73.91	7
	ATOM	1202	C	HIS B 416	-14.560	66.515	29.320	1.00	53.79	6
	ATOM	1203	O	HIS B 416	-14.334	67.477	28.591	1.00	52.81	8
	ATOM	1204	N	PHE B 417	-15.746	65.921	29.372	1.00	48.05	7
	ATOM	1205	CA	PHE B 417	-16.841	66.329	28.505	1.00	47.99	6
30	ATOM	1206	CB	PHE B 417	-18.152	65.694	28.937	1.00	46.11	6
	ATOM	1207	CG	PHE B 417	-19.233	65.781	27.898	1.00	44.27	6
	ATOM	1208	CD1	PHE B 417	-19.280	64.856	26.870	1.00	41.79	6
	ATOM	1209	CD2	PHE B 417	-20.118	66.846	27.893	1.00	40.23	6
	ATOM	1210	CE1	PHE B 417	-20.233	64.959	25.869	1.00	44.30	6
35	ATOM	1211	CE2	PHE B 417	-21.072	66.955	26.893	1.00	36.80	6
	ATOM	1212	CZ	PHE B 417	-21.119	66.016	25.866	1.00	40.69	6
	ATOM	1213	C	PHE B 417	-17.020	67.833	28.423	1.00	46.69	6
	ATOM	1214	O	PHE B 417	-16.799	68.423	27.380	1.00	43.35	8
	ATOM	1215	N	TRP B 418	-17.448	68.452	29.516	1.00	45.14	7
40	ATOM	1216	CA	TRP B 418	-17.681	69.889	29.508	1.00	44.89	6
	ATOM	1217	CB	TRP B 418	-18.045	70.398	30.898	1.00	42.24	6
	ATOM	1218	CG	TRP B 418	-18.162	71.905	31.018	1.00	47.11	6
	ATOM	1219	CD2	TRP B 418	-19.298	72.699	30.620	1.00	46.98	6
	ATOM	1220	CE2	TRP B 418	-18.953	74.061	30.850	1.00	48.94	6
45	ATOM	1221	CE3	TRP B 418	-20.560	72.401	30.086	1.00	45.23	6
	ATOM	1222	CD1	TRP B 418	-17.223	72.778	31.462	1.00	46.24	6
	ATOM	1223	NE1	TRP B 418	-17.690	74.071	31.368	1.00	50.63	7
	ATOM	1224	CZ2	TRP B 418	-19.819	75.109	30.571	1.00	45.46	6
	ATOM	1225	CZ3	TRP B 418	-21.422	73.447	29.809	1.00	44.50	6
50	ATOM	1226	CH2	TRP B 418	-21.065	74.777	30.039	1.00	47.55	6
	ATOM	1227	C	TRP B 418	-16.502	70.662	28.956	1.00	43.88	6
	ATOM	1228	O	TRP B 418	-16.671	71.424	27.986	1.00	43.17	8
	ATOM	1229	N	PRO B 419	-15.292	70.490	29.519	1.00	43.55	7
	ATOM	1230	CD	PRO B 419	-14.967	69.551	30.599	1.00	41.52	6
55	ATOM	1231	CA	PRO B 419	-14.120	71.223	29.011	1.00	41.48	6
	ATOM	1232	CB	PRO B 419	-12.956	70.582	29.724	1.00	39.21	6
	ATOM	1233	CG	PRO B 419	-13.521	69.703	30.774	1.00	39.25	6
	ATOM	1234	C	PRO B 419	-14.035	71.067	27.479	1.00	36.28	6

5	ATOM	1235	O	PRO B 419	-13.690	72.001	26.754	1.00	37.08	8
	ATOM	1236	N	LYS B 420	-14.330	69.871	26.976	1.00	35.96	7
	ATOM	1237	CA	LYS B 420	-14.278	69.609	25.538	1.00	40.82	6
	ATOM	1238	CB	LYS B 420	-14.452	68.103	25.271	1.00	40.78	6
	ATOM	1239	CG	LYS B 420	-13.349	67.214	25.830	1.00	48.62	6
10	ATOM	1240	CD	LYS B 420	-13.565	65.746	25.480	1.00	55.12	6
	ATOM	1241	CE	LYS B 420	-12.427	64.892	26.017	1.00	53.26	6
	ATOM	1242	NZ	LYS B 420	-12.582	63.457	25.608	1.00	52.69	7
	ATOM	1243	C	LYS B 420	-15.414	70.374	24.875	1.00	40.29	6
	ATOM	1244	O	LYS B 420	-15.225	71.015	23.851	1.00	39.66	8
15	ATOM	1245	N	LEU B 421	-16.591	70.300	25.499	1.00	38.33	7
	ATOM	1246	CA	LEU B 421	-17.796	70.958	25.001	1.00	37.60	6
	ATOM	1247	CB	LEU B 421	-18.970	70.702	25.965	1.00	43.66	6
	ATOM	1248	CG	LEU B 421	-20.370	70.850	25.418	1.00	46.50	6
	ATOM	1249	CD1	LEU B 421	-20.529	69.890	24.255	1.00	45.15	6
20	ATOM	1250	CD2	LEU B 421	-21.383	70.538	26.486	1.00	51.31	6
	ATOM	1251	C	LEU B 421	-17.547	72.452	24.823	1.00	39.59	6
	ATOM	1252	O	LEU B 421	-17.975	73.035	23.836	1.00	40.66	8
	ATOM	1253	N	LEU B 422	-16.847	73.059	25.780	1.00	39.57	7
	ATOM	1254	CA	LEU B 422	-16.534	74.478	25.715	1.00	38.63	6
25	ATOM	1255	CB	LEU B 422	-15.829	74.936	26.992	1.00	41.79	6
	ATOM	1256	CG	LEU B 422	-16.714	75.149	28.191	1.00	42.74	6
	ATOM	1257	CD1	LEU B 422	-15.911	75.685	29.360	1.00	42.89	6
	ATOM	1258	CD2	LEU B 422	-17.783	76.162	27.813	1.00	39.27	6
	ATOM	1259	C	LEU B 422	-15.677	74.788	24.513	1.00	40.47	6
30	ATOM	1260	O	LEU B 422	-15.823	75.846	23.917	1.00	47.83	8
	ATOM	1261	N	MET B 423	-14.789	73.853	24.168	1.00	34.27	7
	ATOM	1262	CA	MET B 423	-13.907	74.019	23.024	1.00	35.25	6
	ATOM	1263	CB	MET B 423	-12.920	72.858	22.922	1.00	32.56	6
	ATOM	1264	CG	MET B 423	-12.013	72.703	24.125	1.00	40.70	6
35	ATOM	1265	SD	MET B 423	-10.345	72.007	23.784	1.00	47.65	16
	ATOM	1266	CE	MET B 423	-10.770	70.538	22.761	1.00	47.16	6
	ATOM	1267	C	MET B 423	-14.709	74.100	21.738	1.00	35.13	6
	ATOM	1268	O	MET B 423	-14.341	74.807	20.803	1.00	29.85	8
	ATOM	1269	N	LYS B 424	-15.811	73.361	21.704	1.00	31.56	7
40	ATOM	1270	CA	LYS B 424	-16.676	73.354	20.544	1.00	32.29	6
	ATOM	1271	CB	LYS B 424	-17.783	72.316	20.736	1.00	30.56	6
	ATOM	1272	CG	LYS B 424	-17.257	70.879	20.843	1.00	30.07	6
	ATOM	1273	CD	LYS B 424	-16.444	70.510	19.611	1.00	33.22	6
	ATOM	1274	CE	LYS B 424	-15.795	69.136	19.706	1.00	28.75	6
45	ATOM	1275	NZ	LYS B 424	-14.655	69.067	20.678	1.00	31.01	7
	ATOM	1276	C	LYS B 424	-17.248	74.754	20.304	1.00	29.26	6
	ATOM	1277	O	LYS B 424	-17.439	75.149	19.166	1.00	30.22	8
	ATOM	1278	N	VAL B 425	-17.495	75.499	21.385	1.00	23.53	7
	ATOM	1279	CA	VAL B 425	-18.014	76.852	21.278	1.00	28.91	6
50	ATOM	1280	CB	VAL B 425	-18.278	77.458	22.663	1.00	29.44	6
	ATOM	1281	CG1	VAL B 425	-18.633	78.915	22.547	1.00	28.81	6
	ATOM	1282	CG2	VAL B 425	-19.401	76.733	23.354	1.00	31.22	6
	ATOM	1283	C	VAL B 425	-17.001	77.682	20.498	1.00	32.03	6
	ATOM	1284	O	VAL B 425	-17.368	78.465	19.629	1.00	31.95	8
55	ATOM	1285	N	THR B 426	-15.721	77.508	20.827	1.00	33.61	7
	ATOM	1286	CA	THR B 426	-14.645	78.221	20.137	1.00	30.76	6
	ATOM	1287	CB	THR B 426	-13.270	77.912	20.761	1.00	32.34	6
	ATOM	1288	OG1	THR B 426	-13.073	78.697	21.941	1.00	33.07	8

5	ATOM	1289	CG2	THR	B	426	-12.153	78.174	19.782	1.00	25.40	6
	ATOM	1290	C	THR	B	426	-14.677	77.742	18.706	1.00	32.53	6
	ATOM	1291	O	THR	B	426	-14.639	78.530	17.763	1.00	35.19	8
	ATOM	1292	N	ASP	B	427	-14.749	76.425	18.566	1.00	28.83	7
	ATOM	1293	CA	ASP	B	427	-14.796	75.807	17.257	1.00	35.12	6
10	ATOM	1294	CB	ASP	B	427	-15.096	74.302	17.380	1.00	39.14	6
	ATOM	1295	CG	ASP	B	427	-13.910	73.496	17.806	1.00	45.80	6
	ATOM	1296	OD1	ASP	B	427	-12.786	73.774	17.348	1.00	41.97	8
	ATOM	1297	OD2	ASP	B	427	-14.064	72.517	18.583	1.00	50.06	8
	ATOM	1298	C	ASP	B	427	-15.883	76.502	16.429	1.00	33.94	6
15	ATOM	1299	O	ASP	B	427	-15.673	76.815	15.262	1.00	38.02	8
	ATOM	1300	N	LEU	B	428	-17.040	76.741	17.048	1.00	27.15	7
	ATOM	1301	CA	LEU	B	428	-18.154	77.388	16.367	1.00	29.99	6
	ATOM	1302	CB	LEU	B	428	-19.448	77.190	17.168	1.00	22.49	6
	ATOM	1303	CG	LEU	B	428	-20.086	75.818	17.089	1.00	25.54	6
20	ATOM	1304	CD1	LEU	B	428	-21.282	75.729	18.012	1.00	20.60	6
	ATOM	1305	CD2	LEU	B	428	-20.509	75.564	15.651	1.00	17.24	6
	ATOM	1306	C	LEU	B	428	-17.901	78.863	16.103	1.00	28.94	6
	ATOM	1307	O	LEU	B	428	-18.328	79.388	15.076	1.00	31.26	8
	ATOM	1308	N	ARG	B	429	-17.213	79.524	17.035	1.00	27.64	7
25	ATOM	1309	CA	ARG	B	429	-16.894	80.937	16.883	1.00	28.13	6
	ATOM	1310	CB	ARG	B	429	-16.274	81.507	18.160	1.00	29.59	6
	ATOM	1311	CG	ARG	B	429	-17.246	81.752	19.302	1.00	34.85	6
	ATOM	1312	CD	ARG	B	429	-16.626	82.653	20.372	1.00	47.18	6
	ATOM	1313	NE	ARG	B	429	-17.373	82.714	21.620	1.00	57.93	7
30	ATOM	1314	CZ	ARG	B	429	-18.632	83.124	21.716	1.00	63.62	6
	ATOM	1315	NH1	ARG	B	429	-19.263	83.579	20.622	1.00	60.71	7
	ATOM	1316	NH2	ARG	B	429	-19.238	83.130	22.916	1.00	62.38	7
	ATOM	1317	C	ARG	B	429	-15.930	81.146	15.728	1.00	29.81	6
	ATOM	1318	O	ARG	B	429	-16.101	82.061	14.933	1.00	30.81	8
35	ATOM	1319	N	MET	B	430	-14.908	80.295	15.670	1.00	29.64	7
	ATOM	1320	CA	MET	B	430	-13.920	80.343	14.614	1.00	34.72	6
	ATOM	1321	CB	MET	B	430	-12.939	79.192	14.763	1.00	34.97	6
	ATOM	1322	CG	MET	B	430	-11.787	79.431	15.689	1.00	45.34	6
	ATOM	1323	SD	MET	B	430	-10.729	80.768	15.158	1.00	52.55	16
40	ATOM	1324	CE	MET	B	430	-10.070	80.157	13.610	1.00	55.56	6
	ATOM	1325	C	MET	B	430	-14.638	80.217	13.284	1.00	34.01	6
	ATOM	1326	O	MET	B	430	-14.395	80.996	12.385	1.00	37.29	8
	ATOM	1327	N	ILE	B	431	-15.516	79.217	13.176	1.00	29.99	7
	ATOM	1328	CA	ILE	B	431	-16.296	78.992	11.963	1.00	28.82	6
45	ATOM	1329	CB	ILE	B	431	-17.391	77.929	12.177	1.00	27.39	6
	ATOM	1330	CG2	ILE	B	431	-18.314	77.841	10.959	1.00	23.87	6
	ATOM	1331	CG1	ILE	B	431	-16.784	76.555	12.449	1.00	25.56	6
	ATOM	1332	CD1	ILE	B	431	-17.826	75.464	12.498	1.00	17.29	6
	ATOM	1333	C	ILE	B	431	-16.953	80.288	11.538	1.00	29.49	6
50	ATOM	1334	O	ILE	B	431	-16.837	80.725	10.398	1.00	24.19	8
	ATOM	1335	N	GLY	B	432	-17.657	80.904	12.474	1.00	25.25	7
	ATOM	1336	CA	GLY	B	432	-18.357	82.142	12.179	1.00	30.38	6
	ATOM	1337	C	GLY	B	432	-17.395	83.209	11.725	1.00	32.75	6
	ATOM	1338	O	GLY	B	432	-17.531	83.740	10.637	1.00	36.38	8
55	ATOM	1339	N	ALA	B	433	-16.431	83.522	12.586	1.00	26.77	7
	ATOM	1340	CA	ALA	B	433	-15.407	84.514	12.299	1.00	26.48	6
	ATOM	1341	CB	ALA	B	433	-14.240	84.338	13.253	1.00	19.90	6
	ATOM	1342	C	ALA	B	433	-14.905	84.433	10.867	1.00	30.73	6

5	ATOM	1343	O	ALA	B	433	-14.849	85.432	10.171	1.00	31.60	8
	ATOM	1344	N	CYS	B	434	-14.534	83.246	10.439	1.00	33.22	7
	ATOM	1345	CA	CYS	B	434	-14.023	83.021	9.120	1.00	34.34	6
	ATOM	1346	CB	CYS	B	434	-13.553	81.661	9.226	1.00	35.20	6
	ATOM	1347	SG	CYS	B	434	-12.412	81.249	8.444	1.00	54.48	16
10	ATOM	1348	C	CYS	B	434	-15.106	83.116	8.062	1.00	34.09	6
	ATOM	1349	O	CYS	B	434	-14.844	83.555	6.952	1.00	34.89	8
	ATOM	1350	N	HIS	B	435	-16.318	82.699	8.394	1.00	34.30	7
	ATOM	1351	CA	HIS	B	435	-17.395	82.762	7.443	1.00	35.44	6
	ATOM	1352	CB	HIS	B	435	-18.700	82.404	8.103	1.00	31.76	6
15	ATOM	1353	CG	HIS	B	435	-19.845	82.425	7.149	1.00	32.03	6
	ATOM	1354	CD2	HIS	B	435	-20.483	81.419	6.515	1.00	28.61	6
	ATOM	1355	ND1	HIS	B	435	-20.345	83.600	6.607	1.00	28.48	7
	ATOM	1356	CE1	HIS	B	435	-21.241	83.293	5.672	1.00	33.27	6
	ATOM	1357	NE2	HIS	B	435	-21.341	81.977	5.605	1.00	31.57	7
20	ATOM	1358	C	HIS	B	435	-17.528	84.152	6.878	1.00	32.74	6
	ATOM	1359	O	HIS	B	435	-17.842	84.326	5.715	1.00	32.87	8
	ATOM	1360	N	ALA	B	436	-17.315	85.121	7.758	1.00	31.01	7
	ATOM	1361	CA	ALA	B	436	-17.376	86.520	7.405	1.00	29.91	6
	ATOM	1362	CB	ALA	B	436	-17.008	87.352	8.618	1.00	21.23	6
25	ATOM	1363	C	ALA	B	436	-16.393	86.782	6.266	1.00	33.86	6
	ATOM	1364	O	ALA	B	436	-16.734	87.398	5.257	1.00	36.10	8
	ATOM	1365	N	SER	B	437	-15.162	86.307	6.448	1.00	35.19	7
	ATOM	1366	CA	SER	B	437	-14.122	86.484	5.445	1.00	33.03	6
	ATOM	1367	CB	SER	B	437	-12.882	85.688	5.847	1.00	35.31	6
30	ATOM	1368	OG	SER	B	437	-11.855	85.824	4.879	1.00	44.99	8
	ATOM	1369	C	SER	B	437	-14.642	85.993	4.108	1.00	38.39	6
	ATOM	1370	O	SER	B	437	-14.700	86.730	3.127	1.00	37.54	8
	ATOM	1371	N	ARG	B	438	-15.008	84.719	4.096	1.00	37.32	7
	ATOM	1372	CA	ARG	B	438	-15.526	84.068	2.908	1.00	39.30	6
35	ATOM	1373	CB	ARG	B	438	-16.019	82.660	3.259	1.00	42.97	6
	ATOM	1374	CG	ARG	B	438	-14.910	81.673	3.590	1.00	41.72	6
	ATOM	1375	CD	ARG	B	438	-14.044	81.488	2.356	1.00	45.23	6
	ATOM	1376	NE	ARG	B	438	-14.781	80.936	1.235	1.00	45.66	7
	ATOM	1377	CZ	ARG	B	438	-14.482	81.175	-0.040	1.00	49.71	6
40	ATOM	1378	NH1	ARG	B	438	-13.458	81.977	-0.347	1.00	50.91	7
	ATOM	1379	NH2	ARG	B	438	-15.219	80.619	-1.002	1.00	46.86	7
	ATOM	1380	C	ARG	B	438	-16.659	84.859	2.287	1.00	42.37	6
	ATOM	1381	O	ARG	B	438	-16.841	84.832	1.072	1.00	40.58	8
	ATOM	1382	N	PHE	B	439	-17.417	85.575	3.117	1.00	42.25	7
45	ATOM	1383	CA	PHE	B	439	-18.531	86.354	2.614	1.00	42.81	6
	ATOM	1384	CB	PHE	B	439	-19.198	87.132	3.731	1.00	42.18	6
	ATOM	1385	CG	PHE	B	439	-20.487	87.769	3.323	1.00	42.48	6
	ATOM	1386	CD1	PHE	B	439	-21.535	86.981	2.912	1.00	47.09	6
	ATOM	1387	CD2	PHE	B	439	-20.638	89.141	3.334	1.00	39.76	6
50	ATOM	1388	CE1	PHE	B	439	-22.735	87.543	2.527	1.00	49.17	6
	ATOM	1389	CE2	PHE	B	439	-21.851	89.717	2.944	1.00	45.10	6
	ATOM	1390	CZ	PHE	B	439	-22.901	88.911	2.538	1.00	46.36	6
	ATOM	1391	C	PHE	B	439	-18.016	87.319	1.581	1.00	44.79	6
	ATOM	1392	O	PHE	B	439	-18.514	87.354	0.465	1.00	40.26	8
55	ATOM	1393	N	LEU	B	440	-17.021	88.117	1.987	1.00	42.77	7
	ATOM	1394	CA	LEU	B	440	-16.415	89.115	1.109	1.00	42.96	6
	ATOM	1395	CB	LEU	B	440	-15.169	89.718	1.768	1.00	37.19	6
	ATOM	1396	CG	LEU	B	440	-15.477	90.588	2.967	1.00	36.97	6

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SUBSTITUTE SHEET (RULE 26)

5	ATOM	1397	CD1	LEU	B	440	-14.219	91.838	2.574	1.00	33.65	6
	ATOM	1398	CD2	LEU	B	440	-16.577	91.591	2.574	1.00	35.42	6
	ATOM	1399	C	LEU	B	440	-16.099	88.561	-0.273	1.00	45.47	6
	ATOM	1400	O	LEU	B	440	-16.631	89.059	-1.265	1.00	52.48	8
	ATOM	1401	N	HIS	B	441	-15.238	87.549	-0.345	1.00	49.15	7
10	ATOM	1402	CA	HIS	B	441	-14.929	86.956	-1.632	1.00	54.76	6
	ATOM	1403	CB	HIS	B	441	-14.150	85.700	-1.448	1.00	56.68	6
	ATOM	1404	CG	HIS	B	441	-12.713	85.934	-1.230	1.00	62.73	6
	ATOM	1405	CD2	HIS	B	441	-11.602	85.418	-1.812	1.00	65.73	6
	ATOM	1406	ND1	HIS	B	441	-12.245	86.850	-0.273	1.00	66.01	7
15	ATOM	1407	CE1	HIS	B	441	-10.916	86.847	-0.309	1.00	65.55	6
	ATOM	1408	NE2	HIS	B	441	-10.512	85.993	-1.228	1.00	60.09	7
	ATOM	1409	C	HIS	B	441	-16.217	86.633	-2.301	1.00	55.93	6
	ATOM	1410	O	HIS	B	441	-16.418	86.938	-3.465	1.00	57.33	8
	ATOM	1411	N	MET	B	442	-17.106	85.997	-1.553	1.00	57.81	7
20	ATOM	1412	CA	MET	B	442	-18.399	85.652	-2.106	1.00	59.11	6
	ATOM	1413	CB	MET	B	442	-19.340	85.162	-1.008	1.00	55.93	6
	ATOM	1414	CG	MET	B	442	-18.991	83.796	-0.456	1.00	58.52	6
	ATOM	1415	SD	MET	B	442	-20.310	82.994	0.505	1.00	60.99	16
	ATOM	1416	CE	MET	B	442	-20.525	84.203	1.827	1.00	52.61	6
25	ATOM	1417	C	MET	B	442	-18.991	86.879	-2.785	1.00	60.31	6
	ATOM	1418	O	MET	B	442	-19.646	86.778	-3.817	1.00	58.18	8
	ATOM	1419	N	LYS	B	443	-18.731	88.045	-2.213	1.00	61.45	7
	ATOM	1420	CA	LYS	B	443	-19.267	89.268	-2.758	1.00	64.90	6
	ATOM	1421	CB	LYS	B	443	-19.182	90.358	-1.704	1.00	64.40	6
30	ATOM	1422	CG	LYS	B	443	-20.160	91.449	-1.982	1.00	69.12	6
	ATOM	1423	CD	LYS	B	443	-19.763	92.673	-1.306	1.00	71.14	6
	ATOM	1424	CE	LYS	B	443	-20.508	92.993	-0.491	1.00	73.43	6
	ATOM	1425	NZ	LYS	B	443	-20.174	94.242	0.151	1.00	67.97	7
	ATOM	1426	C	LYS	B	443	-18.528	89.704	-4.020	1.00	67.29	6
35	ATOM	1427	O	LYS	B	443	-18.979	90.586	-4.731	1.00	67.90	8
	ATOM	1428	N	VAL	B	444	-17.383	89.075	-4.285	1.00	66.57	7
	ATOM	1429	CA	VAL	B	444	-16.589	89.418	-5.455	1.00	64.76	6
	ATOM	1430	CB	VAL	B	444	-15.097	89.568	-5.082	1.00	62.76	6
	ATOM	1431	CG1	VAL	B	444	-14.269	89.857	-6.298	1.00	64.00	6
40	ATOM	1432	CG2	VAL	B	444	-14.905	90.678	-4.042	1.00	59.27	6
	ATOM	1433	C	VAL	B	444	-16.800	88.397	-6.569	1.00	68.61	6
	ATOM	1434	O	VAL	B	444	-16.968	88.774	-7.729	1.00	70.60	8
	ATOM	1435	N	GLU	B	445	-16.812	87.118	-6.219	1.00	70.71	7
	ATOM	1436	CA	GLU	B	445	-16.951	86.033	-7.197	1.00	71.45	6
45	ATOM	1437	CB	GLU	B	445	-16.169	84.809	-6.712	1.00	72.36	6
	ATOM	1438	CG	GLU	B	445	-14.736	85.090	-6.392	1.00	40.00	6
	ATOM	1439	CD	GLU	B	445	-13.998	83.890	-5.851	1.00	40.00	6
	ATOM	1440	OE1	GLU	B	445	-14.587	82.798	-5.665	1.00	40.00	8
	ATOM	1441	OE2	GLU	B	445	-12.775	83.995	-5.580	1.00	40.00	8
50	ATOM	1442	C	GLU	B	445	-18.375	85.574	-7.422	1.00	71.46	6
	ATOM	1443	O	GLU	B	445	-18.605	84.542	-8.064	1.00	73.02	8
	ATOM	1444	N	CYS	B	446	-19.328	86.333	-6.900	1.00	71.12	7
	ATOM	1445	CA	CYS	B	446	-20.694	85.942	-7.062	1.00	70.83	6
	ATOM	1446	CB	CYS	B	446	-21.196	85.230	-5.784	1.00	71.05	6
55	ATOM	1447	SG	CYS	B	446	-20.296	83.720	-5.349	1.00	72.83	16
	ATOM	1448	C	CYS	B	446	-21.563	87.135	-7.386	1.00	71.91	6
	ATOM	1449	O	CYS	B	446	-21.307	88.244	-6.911	1.00	72.06	8
	ATOM	1450	N	PRO	B	447	-22.550	86.928	-8.256	1.00	73.12	7



5	ATOM	1451	CD	PRO B 447	-22.837	85.637	-8.886	1.00	72.88	6
	ATOM	1452	CA	PRO B 447	-23.461	87.997	-8.653	1.00	74.22	6
	ATOM	1453	CB	PRO B 447	-24.399	87.338	-9.659	1.00	72.98	6
	ATOM	1454	CG	PRO B 447	-23.981	85.934	-9.776	1.00	74.77	6
	ATOM	1455	C	PRO B 447	-24.203	88.519	-7.451	1.00	75.94	6
10	ATOM	1456	O	PRO B 447	-24.601	87.749	-6.611	1.00	76.67	8
	ATOM	1457	N	THR B 448	-24.390	89.828	-7.373	1.00	76.91	7
	ATOM	1458	CA	THR B 448	-25.134	90.436	-6.268	1.00	78.24	6
	ATOM	1459	CB	THR B 448	-24.883	91.948	-6.276	1.00	81.33	6
	ATOM	1460	OG1	THR B 448	-25.474	92.525	-7.451	1.00	84.46	8
15	ATOM	1461	CG2	THR B 448	-23.394	92.234	-6.269	1.00	83.51	6
	ATOM	1462	C	THR B 448	-26.594	90.160	-6.619	1.00	77.42	6
	ATOM	1463	O	THR B 448	-27.512	90.649	-5.982	1.00	77.65	8
	ATOM	1464	N	GLU B 449	-26.759	89.400	-7.697	1.00	76.29	7
	ATOM	1465	CA	GLU B 449	-28.051	89.017	-8.211	1.00	75.03	6
20	ATOM	1466	CB	GLU B 449	-27.923	88.915	-9.719	1.00	74.62	6
	ATOM	1467	CG	GLU B 449	-28.823	87.966	-10.343	1.00	40.00	6
	ATOM	1468	CD	GLU B 449	-28.522	87.831	-11.756	1.00	40.00	6
	ATOM	1469	OE1	GLU B 449	-27.366	88.072	-12.190	1.00	40.00	8
	ATOM	1470	OE2	GLU B 449	-29.449	87.438	-12.492	1.00	40.00	8
25	ATOM	1471	C	GLU B 449	-28.448	87.660	-7.609	1.00	73.49	6
	ATOM	1472	O	GLU B 449	-29.479	87.092	-7.953	1.00	70.24	8
	ATOM	1473	N	LEU B 450	-27.624	87.158	-6.695	1.00	70.80	7
	ATOM	1474	CA	LEU B 450	-27.879	85.879	-6.058	1.00	68.82	6
	ATOM	1475	CB	LEU B 450	-26.772	84.887	-6.447	1.00	71.91	6
30	ATOM	1476	CG	LEU B 450	-26.612	84.503	-7.900	1.00	76.62	6
	ATOM	1477	CD1	LEU B 450	-25.396	83.637	-8.059	1.00	77.95	6
	ATOM	1478	CD2	LEU B 450	-27.849	83.775	-8.351	1.00	76.46	6
	ATOM	1479	C	LEU B 450	-27.941	86.012	-4.536	1.00	66.22	6
	ATOM	1480	O	LEU B 450	-28.251	85.039	-3.849	1.00	66.01	8
35	ATOM	1481	N	PHE B 451	-27.666	87.215	-4.012	1.00	61.96	7
	ATOM	1482	CA	PHE B 451	-27.635	87.494	-2.585	1.00	58.44	6
	ATOM	1483	CB	PHE B 451	-26.579	88.573	-2.263	1.00	61.34	6
	ATOM	1484	CG	PHE B 451	-25.153	88.078	-2.413	1.00	63.02	6
	ATOM	1485	CD1	PHE B 451	-24.675	87.587	-3.626	1.00	62.92	6
40	ATOM	1486	CD2	PHE B 451	-24.283	88.173	-1.346	1.00	63.07	6
	ATOM	1487	CE1	PHE B 451	-23.327	87.217	-3.757	1.00	65.12	6
	ATOM	1488	CE2	PHE B 451	-22.939	87.806	-1.472	1.00	64.66	6
	ATOM	1489	CZ	PHE B 451	-22.459	87.335	-2.686	1.00	67.12	6
	ATOM	1490	C	PHE B 451	-28.931	87.994	-1.962	1.00	56.41	6
45	ATOM	1491	O	PHE B 451	-29.207	89.214	-1.908	1.00	56.56	8
	ATOM	1492	N	PRO B 452	-29.791	87.072	-1.473	1.00	53.28	7
	ATOM	1493	CD	PRO B 452	-29.767	85.611	-1.494	1.00	50.46	6
	ATOM	1494	CA	PRO B 452	-31.037	87.598	-0.843	1.00	50.26	6
	ATOM	1495	CB	PRO B 452	-31.746	86.375	-0.301	1.00	49.19	6
50	ATOM	1496	CG	PRO B 452	-31.024	85.197	-0.842	1.00	45.89	6
	ATOM	1497	C	PRO B 452	-30.636	88.567	0.251	1.00	49.62	6
	ATOM	1498	O	PRO B 452	-29.628	88.401	0.906	1.00	52.35	8
	ATOM	1499	N	PRO B 453	-31.494	89.539	0.535	1.00	51.50	7
	ATOM	1500	CD	PRO B 453	-32.853	89.644	0.022	1.00	49.66	6
55	ATOM	1501	CA	PRO B 453	-31.184	90.573	1.530	1.00	50.89	6
	ATOM	1502	CB	PRO B 453	-32.422	91.401	1.625	1.00	51.49	6
	ATOM	1503	CG	PRO B 453	-33.378	90.827	0.724	1.00	50.82	6
	ATOM	1504	C	PRO B 453	-30.829	90.039	2.906	1.00	50.99	6

5	ATOM	1505	O	PRO B 453	-29.700	90.206	3.345	1.00	54.17	8
	ATOM	1506	N	LEU B 454	-31.807	89.458	3.631	1.00	51.21	7
	ATOM	1507	CA	LEU B 454	-31.538	88.945	4.948	1.00	47.17	6
	ATOM	1508	CB	LEU B 454	-32.550	87.858	5.330	1.00	44.44	6
	ATOM	1509	CG	LEU B 454	-32.347	87.412	6.748	1.00	41.33	6
10	ATOM	1510	CD1	LEU B 454	-31.987	88.589	7.631	1.00	35.93	6
	ATOM	1511	CD2	LEU B 454	-33.590	86.732	7.239	1.00	34.79	6
	ATOM	1512	C	LEU B 454	-30.099	88.443	4.928	1.00	42.25	6
	ATOM	1513	O	LEU B 454	-29.323	88.774	5.812	1.00	40.82	8
	ATOM	1514	N	PHE B 455	-29.716	87.707	3.885	1.00	39.29	7
15	ATOM	1515	CA	PHE B 455	-28.347	87.204	3.770	1.00	41.81	6
	ATOM	1516	CB	PHE B 455	-28.132	86.536	2.418	1.00	47.22	6
	ATOM	1517	CG	PHE B 455	-26.813	85.836	2.292	1.00	56.97	6
	ATOM	1518	CD1	PHE B 455	-26.437	84.915	3.247	1.00	57.23	6
	ATOM	1519	CD2	PHE B 455	-25.949	86.094	1.236	1.00	59.40	6
20	ATOM	1520	CE1	PHE B 455	-25.225	84.234	3.153	1.00	56.58	6
	ATOM	1521	CE2	PHE B 455	-24.720	85.409	1.134	1.00	61.80	6
	ATOM	1522	CZ	PHE B 455	-24.360	84.481	2.103	1.00	59.94	6
	ATOM	1523	C	PHE B 455	-27.400	88.386	3.923	1.00	45.12	6
	ATOM	1524	O	PHE B 455	-26.657	88.450	4.889	1.00	39.95	8
25	ATOM	1525	N	LEU B 456	-27.439	89.303	2.949	1.00	43.92	7
	ATOM	1526	CA	LEU B 456	-26.597	90.503	2.947	1.00	44.08	6
	ATOM	1527	CB	LEU B 456	-27.001	91.440	1.802	1.00	50.20	6
	ATOM	1528	CG	LEU B 456	-26.439	91.155	0.432	1.00	55.79	6
	ATOM	1529	CD1	LEU B 456	-27.064	92.082	-0.591	1.00	54.70	6
30	ATOM	1530	CD2	LEU B 456	-24.920	91.345	0.494	1.00	53.01	6
	ATOM	1531	C	LEU B 456	-26.689	91.245	4.264	1.00	44.65	6
	ATOM	1532	O	LEU B 456	-25.678	91.540	4.886	1.00	45.93	8
	ATOM	1533	N	GLU B 457	-27.990	91.268	4.265	1.00	44.56	7
	ATOM	1534	CA	GLU B 457	-28.288	92.016	5.497	1.00	46.37	6
35	ATOM	1535	C	GLU B 457	-27.434	91.452	6.628	1.00	43.60	6
	ATOM	1536	O	GLU B 457	-26.754	92.223	7.339	1.00	42.69	8
	ATOM	1537	CB	GLU B 457	-29.769	91.879	5.855	1.00	50.16	6
	ATOM	1538	CG	GLU B 457	-30.208	92.849	6.954	1.00	20.00	6
	ATOM	1539	CD	GLU B 457	-31.646	93.338	6.782	1.00	20.00	6
40	ATOM	1540	OE1	GLU B 457	-32.351	92.932	5.779	1.00	20.00	8
	ATOM	1541	OE2	GLU B 457	-32.157	94.156	7.638	1.00	20.00	8
	ATOM	1542	N	VAL B 458	-27.428	90.413	7.281	1.00	43.21	7
	ATOM	1543	CA	VAL B 458	-26.706	89.739	8.351	1.00	44.98	6
	ATOM	1544	CB	VAL B 458	-27.075	88.255	8.432	1.00	44.83	6
45	ATOM	1545	CG1	VAL B 458	-26.440	87.623	9.646	1.00	49.72	6
	ATOM	1546	CG2	VAL B 458	-28.562	88.086	8.474	1.00	40.89	6
	ATOM	1547	C	VAL B 458	-25.190	89.822	8.311	1.00	42.72	6
	ATOM	1548	O	VAL B 458	-24.551	90.179	9.303	1.00	42.88	8
	ATOM	1549	N	PHE B 459	-24.605	89.488	7.180	1.00	44.53	7
50	ATOM	1550	CA	PHE B 459	-23.165	89.480	7.077	1.00	48.18	6
	ATOM	1551	CB	PHE B 459	-22.747	88.457	6.065	1.00	43.60	6
	ATOM	1552	CG	PHE B 459	-23.167	87.116	6.441	1.00	40.79	6
	ATOM	1553	CD1	PHE B 459	-24.494	86.750	6.368	1.00	41.01	6
	ATOM	1554	CD2	PHE B 459	-22.263	86.286	7.009	1.00	39.48	6
55	ATOM	1555	CE1	PHE B 459	-24.892	85.540	6.889	1.00	40.62	6
	ATOM	1556	CE2	PHE B 459	-22.649	85.091	7.527	1.00	36.87	6
	ATOM	1557	CZ	PHE B 459	-23.967	84.711	7.455	1.00	36.39	6
	ATOM	1558	C	PHE B 459	-22.627	90.758	6.623	1.00	52.71	6

5	ATOM	1559	O	PHE	B	459	-21.414	91.050	6.791	1.00	51.34	8
	ATOM	1560	N	GLU	B	460	-23.489	91.531	5.976	1.00	62.92	7
	ATOM	1561	CA	GLU	B	460	-22.953	92.741	5.533	1.00	69.33	6
	ATOM	1562	CB	GLU	B	460	-23.851	93.487	4.505	1.00	72.95	6
	ATOM	1563	CG	GLU	B	460	-22.917	94.002	3.412	1.00	78.35	6
10	ATOM	1564	CD	GLU	B	460	-22.908	95.480	3.256	1.00	82.97	6
	ATOM	1565	OE1	GLU	B	460	-23.257	96.213	4.217	1.00	88.28	8
	ATOM	1566	OE2	GLU	B	460	-22.524	95.977	2.167	1.00	84.80	8
	ATOM	1567	C	GLU	B	460	-22.790	93.576	6.786	1.00	71.87	6
	ATOM	1568	O	GLU	B	460	-23.471	93.391	7.802	1.00	74.51	8
15	ATOM	1569	N	ASP	B	461	-21.796	94.449	6.696	1.00	78.50	7
	ATOM	1570	CA	ASP	B	461	-21.401	95.328	7.701	1.00	84.19	6
	ATOM	1571	CB	ASP	B	461	-20.182	96.032	7.125	1.00	85.82	6
	ATOM	1572	CG	ASP	B	461	-19.261	95.066	6.463	1.00	89.62	6
	ATOM	1573	OD1	ASP	B	461	-19.670	93.929	5.982	1.00	93.00	8
20	ATOM	1574	OD2	ASP	B	461	-18.084	95.361	6.387	1.00	93.04	8
	ATOM	1575	C	ASP	B	461	-22.540	96.291	8.012	1.00	86.80	6
	ATOM	1576	O	ASP	B	461	-23.063	96.176	9.139	1.00	88.70	8
	ATOM	1577	OXT	ASP	B	461	-22.962	97.048	7.098	1.00	88.70	8
	TER											
25	ATOM	4002	C1	T3	J	1	20.152	36.643	29.561	1.00	22.34	6
	ATOM	4003	C2	T3	J	1	19.021	41.567	29.283	1.00	21.84	6
	ATOM	4004	C3	T3	J	1	18.880	37.086	29.226	1.00	23.43	6
	ATOM	4005	C4	T3	J	1	18.249	42.606	28.776	1.00	22.31	6
	ATOM	4006	C5	T3	J	1	18.747	38.372	28.866	1.00	24.83	6
30	ATOM	4007	C6	T3	J	1	17.938	43.621	29.664	1.00	25.16	6
	ATOM	4008	C7	T3	J	1	19.799	39.296	28.753	1.00	24.65	6
	ATOM	4009	C8	T3	J	1	18.330	43.594	31.028	1.00	21.93	6
	ATOM	4010	C9	T3	J	1	21.101	38.940	29.075	1.00	25.09	6
	ATOM	4011	C10	T3	J	1	19.063	42.558	31.465	1.00	23.66	6
35	ATOM	4012	C11	T3	J	1	21.254	37.600	29.456	1.00	23.12	6
	ATOM	4013	C12	T3	J	1	19.459	41.490	30.621	1.00	19.67	6
	ATOM	4014	C13	T3	J	1	20.370	35.228	30.075	1.00	18.97	6
	ATOM	4015	C15	T3	J	1	21.549	34.480	29.455	1.00	19.32	6
	ATOM	4016	C17	T3	J	1	21.535	33.003	29.710	1.00	19.02	6
40	ATOM	4017	I1	T3	J	1	16.898	39.029	28.661	1.00	25.29	53
	ATOM	4018	I2	T3	J	1	17.058	45.327	29.154	1.00	26.49	53
	ATOM	4019	I3	T3	J	1	22.763	40.262	29.169	1.00	25.67	53
	ATOM	4020	N1	T3	J	1	21.800	34.859	28.024	1.00	15.12	7
	ATOM	4021	O1	T3	J	1	17.934	44.682	31.806	1.00	21.79	8
45	ATOM	4022	O2	T3	J	1	19.432	40.560	28.362	1.00	22.05	8
	ATOM	4023	O3	T3	J	1	21.911	32.260	28.776	1.00	20.38	8
	ATOM	4024	O4	T3	J	1	21.137	32.622	30.840	1.00	20.16	8
	TER											
	ATOM	4025	C1	T3	K	1	-28.131	75.928	7.543	1.00	22.34	6
50	ATOM	4026	C2	T3	K	1	-24.676	77.673	4.318	1.00	21.84	6
	ATOM	4027	C3	T3	K	1	-28.490	76.351	6.201	1.00	23.43	6
	ATOM	4028	C4	T3	K	1	-24.217	77.893	2.989	1.00	22.31	6
	ATOM	4029	C5	T3	K	1	-27.485	76.499	5.233	1.00	24.83	6
	ATOM	4030	C6	T3	K	1	-23.545	79.124	2.700	1.00	25.16	6
55	ATOM	4031	C7	T3	K	1	-26.132	76.227	5.581	1.00	24.65	6
	ATOM	4032	C8	T3	K	1	-23.382	80.104	3.772	1.00	21.93	6
	ATOM	4033	C9	T3	K	1	-25.685	75.833	6.855	1.00	25.09	6
	ATOM	4034	C10	T3	K	1	-23.867	79.823	5.042	1.00	23.66	6

5	ATOM	4035	C11	T3	K	1	-26.708	75.670	7.834	1.00	23.12	6
	ATOM	4036	C12	T3	K	1	-24.521	78.610	5.376	1.00	19.67	6
	ATOM	4037	C13	T3	K	1	-29.211	75.830	8.626	1.00	18.97	6
	ATOM	4038	C15	T3	K	1	-29.181	74.567	9.488	1.00	19.32	6
	ATOM	4039	C17	T3	K	1	-30.440	74.343	10.264	1.00	19.02	6
10	ATOM	4040	I1	T3	K	1	-27.868	77.342	3.316	1.00	25.29	53
	ATOM	4041	I2	T3	K	1	-22.732	79.619	0.850	1.00	26.49	53
	ATOM	4042	I3	T3	K	1	-23.602	75.792	7.334	1.00	25.67	53
	ATOM	4043	N1	T3	K	1	-28.680	73.342	8.762	1.00	15.12	7
	ATOM	4044	O1	T3	K	1	-22.742	81.265	3.443	1.00	21.79	8
15	ATOM	4045	O2	T3	K	1	-25.267	76.388	4.595	1.00	22.05	8
	ATOM	4046	O3	T3	K	1	-30.816	73.159	10.382	1.00	20.38	8
	ATOM	4047	O4	T3	K	1	-31.028	75.359	10.729	1.00	20.16	8
	TER											
	ATOM	1	C	LYS	X	686	13.868	40.176	48.888	1.00	40.00	6
20	ATOM	2	O	LYS	X	686	13.914	40.120	47.639	1.00	40.00	8
	ATOM	3	N	LYS	X	686	14.374	42.245	50.489	1.00	40.00	7
	ATOM	4	CA	LYS	X	686	14.937	41.070	49.710	1.00	40.00	6
	ATOM	5	N	HIS	X	687	13.038	39.527	49.705	1.00	40.00	7
	ATOM	6	CA	HIS	X	687	11.891	38.518	49.521	1.00	40.00	6
25	ATOM	7	CB	HIS	X	687	10.639	39.000	50.212	1.00	40.00	6
	ATOM	8	CG	HIS	X	687	10.981	39.526	51.563	1.00	40.00	6
	ATOM	9	CD2	HIS	X	687	11.021	38.908	52.753	1.00	40.00	6
	ATOM	10	ND1	HIS	X	687	11.354	40.844	51.754	1.00	40.00	7
	ATOM	11	CE1	HIS	X	687	11.614	40.994	53.034	1.00	40.00	6
30	ATOM	12	NE2	HIS	X	687	11.422	39.847	53.646	1.00	40.00	7
	ATOM	13	C	HIS	X	687	11.183	38.108	48.208	1.00	40.00	6
	ATOM	14	O	HIS	X	687	11.674	38.361	47.094	1.00	40.00	8
	ATOM	15	N	LYS	X	688	10.064	37.458	48.649	1.00	40.00	7
	ATOM	16	CA	LYS	X	688	8.911	36.858	47.931	1.00	40.00	6
35	ATOM	17	CB	LYS	X	688	8.292	37.850	46.968	1.00	40.00	6
	ATOM	18	C	LYS	X	688	9.246	35.573	47.161	1.00	40.00	6
	ATOM	19	O	LYS	X	688	9.319	34.473	47.722	1.00	40.00	8
	ATOM	20	N	ILE	X	689	9.426	35.754	45.865	1.00	40.00	7
	ATOM	21	CA	ILE	X	689	9.661	34.640	44.924	1.00	40.00	6
40	ATOM	22	CB	ILE	X	689	9.731	35.167	43.498	1.00	40.00	6
	ATOM	23	CG2	ILE	X	689	9.638	34.053	42.453	1.00	40.00	6
	ATOM	24	CG1	ILE	X	689	8.597	36.141	43.176	1.00	40.00	6
	ATOM	25	CD1	ILE	X	689	8.250	36.183	41.688	1.00	40.00	6
	ATOM	26	C	ILE	X	689	10.954	33.869	45.228	1.00	40.00	6
45	ATOM	27	O	ILE	X	689	10.920	32.657	45.511	1.00	40.00	8
	ATOM	28	N	LEU	X	690	12.065	34.579	45.140	1.00	40.00	7
	ATOM	29	CA	LEU	X	690	13.391	33.996	45.397	1.00	40.00	6
	ATOM	30	CB	LEU	X	690	14.349	35.043	45.892	1.00	40.00	6
	ATOM	31	CG	LEU	X	690	14.450	36.168	44.906	1.00	40.00	6
50	ATOM	32	CD1	LEU	X	690	15.397	37.261	45.363	1.00	40.00	6
	ATOM	33	CD2	LEU	X	690	14.940	35.695	43.540	1.00	40.00	6
	ATOM	34	C	LEU	X	690	13.271	32.999	46.466	1.00	40.00	6
	ATOM	35	O	LEU	X	690	13.633	31.832	46.315	1.00	40.00	8
	ATOM	36	N	HIS	X	691	12.773	33.472	47.541	1.00	40.00	7
55	ATOM	37	CA	HIS	X	691	12.557	32.559	48.569	1.00	40.00	6
	ATOM	38	CB	HIS	X	691	11.729	33.212	49.658	1.00	40.00	6
	ATOM	39	CG	HIS	X	691	12.588	34.116	50.564	1.00	40.00	6
	ATOM	40	CD2	HIS	X	691	13.648	33.852	51.385	1.00	40.00	6
	ATOM											

5	ATOM	41	ND1	HIS	X	691	12.359	35.484	50.669	1.00	40.00	7
	ATOM	42	CE1	HIS	X	691	13.242	35.991	51.513	1.00	40.00	6
	ATOM	43	NE2	HIS	X	691	14.016	35.031	51.949	1.00	40.00	7
	ATOM	44	C	HIS	X	691	11.954	31.331	47.861	1.00	40.00	6
	ATOM	45	O	HIS	X	691	12.505	30.240	47.882	1.00	40.00	8
10	ATOM	46	N	ARG	X	692	10.839	31.494	47.167	1.00	40.00	7
	ATOM	47	CA	ARG	X	692	10.169	30.333	46.518	1.00	40.00	6
	ATOM	48	CB	ARG	X	692	9.118	30.800	45.517	1.00	40.00	6
	ATOM	49	C	ARG	X	692	11.153	29.402	45.752	1.00	40.00	6
	ATOM	50	O	ARG	X	692	11.030	28.168	45.779	1.00	40.00	8
15	ATOM	51	N	LEU	X	693	12.117	30.000	45.072	1.00	40.00	7
	ATOM	52	CA	LEU	X	693	13.078	29.252	44.226	1.00	40.00	6
	ATOM	53	CB	LEU	X	693	13.784	30.210	43.274	1.00	40.00	6
	ATOM	54	CG	LEU	X	693	12.796	31.012	42.432	1.00	40.00	6
	ATOM	55	CD1	LEU	X	693	13.479	31.969	41.458	1.00	40.00	6
20	ATOM	56	CD2	LEU	X	693	11.884	30.126	41.579	1.00	40.00	6
	ATOM	57	C	LEU	X	693	14.143	28.531	45.054	1.00	40.00	6
	ATOM	58	O	LEU	X	693	14.702	27.508	44.633	1.00	40.00	8
	ATOM	59	N	LEU	X	694	14.400	29.079	46.209	1.00	40.00	7
	ATOM	60	CA	LEU	X	694	15.407	28.538	47.115	1.00	40.00	6
25	ATOM	61	CB	LEU	X	694	15.871	29.626	48.084	1.00	40.00	6
	ATOM	62	CG	LEU	X	694	16.692	30.716	47.404	1.00	40.00	6
	ATOM	63	CD1	LEU	X	694	17.279	31.724	48.391	1.00	40.00	6
	ATOM	64	CD2	LEU	X	694	17.879	30.156	46.619	1.00	40.00	6
	ATOM	65	C	LEU	X	694	14.837	27.404	47.957	1.00	40.00	6
30	ATOM	66	O	LEU	X	694	15.555	26.747	48.716	1.00	40.00	8
	ATOM	67	N	GLN	X	695	13.554	27.157	47.809	1.00	40.00	7
	ATOM	68	CA	GLN	X	695	12.883	26.188	48.685	1.00	40.00	6
	ATOM	69	C	GLN	X	695	12.423	24.910	47.977	1.00	40.00	6
	ATOM	70	O	GLN	X	695	12.309	23.845	48.598	1.00	40.00	8
35	ATOM	71	CB	GLN	X	695	11.681	26.858	49.322	1.00	40.00	6
	ATOM	72	CG	GLN	X	695	12.074	28.125	50.080	1.00	20.00	6
	ATOM	73	CD	GLN	X	695	10.899	28.768	50.801	1.00	20.00	6
	ATOM	74	OE1	GLN	X	695	9.772	28.296	50.671	1.00	20.00	8
	ATOM	75	NE2	GLN	X	695	11.092	29.828	51.560	1.00	20.00	7
40	ATOM	76	N	ASP	X	696	12.155	25.020	46.714	1.00	40.00	7
	ATOM	77	CA	ASP	X	696	11.698	23.885	45.910	1.00	40.00	6
	ATOM	78	CB	ASP	X	696	11.450	24.400	44.497	1.00	40.00	6
	ATOM	79	CG	ASP	X	696	10.782	23.411	43.548	1.00	40.00	6
	ATOM	80	OD1	ASP	X	696	10.550	22.203	43.920	1.00	40.00	8
45	ATOM	81	OD2	ASP	X	696	10.449	23.804	42.362	1.00	40.00	8
	ATOM	82	C	ASP	X	696	12.774	22.806	45.876	1.00	40.00	6
	ATOM	83	O	ASP	X	696	13.937	23.077	45.562	1.00	40.00	8
	ATOM	84	N	SER	X	697	12.370	21.610	46.213	1.00	40.00	7
	ATOM	85	CA	SER	X	697	13.258	20.453	46.128	1.00	40.00	6
50	ATOM	86	CB	SER	X	697	12.685	19.371	47.049	1.00	40.00	6
	ATOM	87	OG	SER	X	697	12.535	19.899	48.374	1.00	40.00	8
	ATOM	88	C	SER	X	697	13.329	20.130	44.613	1.00	40.00	6
	ATOM	89	O	SER	X	697	14.247	20.573	43.914	1.00	40.00	8
	ATOM	90	N	SER	X	698	12.355	19.357	44.183	1.00	40.00	7
55	ATOM	91	CA	SER	X	698	11.985	19.100	42.752	1.00	40.00	6
	ATOM	92	CB	SER	X	698	11.693	20.417	42.036	1.00	40.00	6
	ATOM	93	OG	SER	X	698	10.510	21.000	42.577	1.00	40.00	8
	ATOM	94	C	SER	X	698	12.887	18.340	41.758	1.00	40.00	6

5	ATOM	95	O	SER X	698	13.253	17.158	42.026	1.00	40.00	8
	ATOM	96	OXT	SER X	698	13.131	18.976	40.714	1.00	40.00	8
	TER										
	ATOM	1	CB	LYS Y	688	-33.793	96.885	6.491	1.00	40.00	6
	ATOM	2	C	LYS Y	688	-35.002	95.370	8.130	1.00	40.00	6
10	ATOM	3	O	LYS Y	688	-36.027	95.520	8.779	1.00	40.00	8
	ATOM	4	N	LYS Y	688	-32.717	96.619	8.695	1.00	40.00	7
	ATOM	5	CA	LYS Y	688	-34.040	96.591	7.954	1.00	40.00	6
	ATOM	6	N	ILE Y	689	-34.578	93.781	6.908	1.00	40.00	7
	ATOM	7	CA	ILE Y	689	-35.862	93.106	7.268	1.00	40.00	6
15	ATOM	8	CB	ILE Y	689	-35.971	91.759	6.572	1.00	40.00	6
	ATOM	9	CG2	ILE Y	689	-37.270	91.077	6.932	1.00	40.00	6
	ATOM	10	CG1	ILE Y	689	-35.917	91.937	5.062	1.00	40.00	6
	ATOM	11	CD1	ILE Y	689	-36.341	90.691	4.289	1.00	40.00	6
	ATOM	12	C	ILE Y	689	-36.032	92.870	8.780	1.00	40.00	6
20	ATOM	13	O	ILE Y	689	-36.913	93.446	9.442	1.00	40.00	8
	ATOM	14	N	LEU Y	690	-35.019	92.834	9.787	1.00	40.00	7
	ATOM	15	CA	LEU Y	690	-34.956	92.320	11.163	1.00	40.00	6
	ATOM	16	CB	LEU Y	690	-33.528	92.432	11.697	1.00	40.00	6
	ATOM	17	CG	LEU Y	690	-32.516	91.647	10.864	1.00	40.00	6
25	ATOM	18	CD1	LEU Y	690	-31.087	91.764	11.397	1.00	40.00	6
	ATOM	19	CD2	LEU Y	690	-32.819	90.148	10.812	1.00	40.00	6
	ATOM	20	C	LEU Y	690	-35.899	93.123	12.065	1.00	40.00	6
	ATOM	21	O	LEU Y	690	-36.570	92.492	12.928	1.00	40.00	8
	ATOM	22	N	HIS Y	691	-36.039	94.731	11.373	1.00	40.00	7
30	ATOM	23	CA	HIS Y	691	-36.634	94.923	12.683	1.00	40.00	6
	ATOM	24	CB	HIS Y	691	-36.854	96.383	12.935	1.00	40.00	6
	ATOM	25	CG	HIS Y	691	-35.610	97.153	13.078	1.00	40.00	6
	ATOM	26	CD2	HIS Y	691	-34.757	97.640	12.159	1.00	40.00	6
	ATOM	27	ND1	HIS Y	691	-35.129	97.579	14.319	1.00	40.00	7
35	ATOM	28	CE1	HIS Y	691	-34.039	98.290	14.122	1.00	40.00	6
	ATOM	29	NE2	HIS Y	691	-33.786	98.346	12.815	1.00	40.00	7
	ATOM	30	C	HIS Y	691	-37.972	94.287	12.756	1.00	40.00	6
	ATOM	31	O	HIS Y	691	-38.240	93.417	13.545	1.00	40.00	8
	ATOM	32	N	ARG Y	692	-38.265	94.388	11.505	1.00	40.00	7
40	ATOM	33	CA	ARG Y	692	-39.577	93.869	11.276	1.00	40.00	6
	ATOM	34	CB	ARG Y	692	-39.653	93.692	9.795	1.00	40.00	6
	ATOM	35	CG	ARG Y	692	-40.759	92.764	9.329	1.00	40.00	6
	ATOM	36	CD	ARG Y	692	-40.618	92.422	7.848	1.00	40.00	6
	ATOM	37	NE	ARG Y	692	-41.849	92.641	7.091	1.00	40.00	7
45	ATOM	38	CZ	ARG Y	692	-41.898	92.758	5.763	1.00	40.00	6
	ATOM	39	NH1	ARG Y	692	-40.784	92.695	5.024	1.00	40.00	7
	ATOM	40	NH2	ARG Y	692	-43.034	92.940	5.080	1.00	40.00	7
	ATOM	41	C	ARG Y	692	-39.941	92.547	11.995	1.00	40.00	6
	ATOM	42	O	ARG Y	692	-41.001	92.440	12.649	1.00	40.00	8
50	ATOM	43	N	LEU Y	693	-39.095	91.576	11.816	1.00	40.00	7
	ATOM	44	CA	LEU Y	693	-39.230	90.232	12.395	1.00	40.00	6
	ATOM	45	CB	LEU Y	693	-38.362	89.337	11.615	1.00	40.00	6
	ATOM	46	CG	LEU Y	693	-38.737	89.375	10.132	1.00	40.00	6
	ATOM	47	CD1	LEU Y	693	-37.794	88.570	9.247	1.00	40.00	6
55	ATOM	48	CD2	LEU Y	693	-40.142	88.827	9.862	1.00	40.00	6
	ATOM	49	C	LEU Y	693	-38.921	90.378	13.816	1.00	40.00	6
	ATOM	50	O	LEU Y	693	-39.191	89.474	14.615	1.00	40.00	8
	ATOM	51	N	LEU Y	694	-38.366	91.533	14.076	1.00	40.00	7

5	ATOM	52	CA	LEU	Y	694	-38.174	91.885	15.435	1.00	40.00	6
	ATOM	53	CB	LEU	Y	694	-37.181	93.002	15.561	1.00	40.00	6
	ATOM	54	CG	LEU	Y	694	-35.799	92.377	15.869	1.00	40.00	6
	ATOM	55	CD1	LEU	Y	694	-34.897	93.275	16.702	1.00	40.00	6
	ATOM	56	CD2	LEU	Y	694	-35.897	91.055	16.661	1.00	40.00	6
10	ATOM	57	C	LEU	Y	694	-39.596	91.903	15.915	1.00	40.00	6
	ATOM	58	O	LEU	Y	694	-39.985	91.253	16.858	1.00	40.00	8
	ATOM	59	N	GLN	Y	695	-40.787	92.229	15.048	1.00	40.00	7
	ATOM	60	CA	GLN	Y	695	-42.034	91.457	15.543	1.00	40.00	6
	ATOM	61	C	GLN	Y	695	-43.054	90.901	14.240	1.00	40.00	6
15	ATOM	62	O	GLN	Y	695	-43.102	91.557	13.189	1.00	40.00	8
	ATOM	63	CB	GLN	Y	695	-42.362	92.025	16.923	1.00	40.00	6
	ATOM	64	CG	GLN	Y	695	-41.013	92.101	17.768	1.00	40.00	6
	ATOM	65	CD	GLN	Y	695	-40.943	91.235	19.059	1.00	40.00	6
	ATOM	66	OE1	GLN	Y	695	-41.828	90.426	19.318	1.00	40.00	8
20	ATOM	67	NE2	GLN	Y	695	-39.938	91.399	19.916	1.00	40.00	7
	ATOM	68	N	ASP	Y	696	-43.802	89.498	14.402	1.00	40.00	7
	ATOM	69	CA	ASP	Y	696	-44.784	88.354	13.428	1.00	40.00	6
	ATOM	70	C	ASP	Y	696	-46.034	88.934	12.759	1.00	40.00	6
	ATOM	71	O	ASP	Y	696	-46.266	88.655	11.529	1.00	40.00	8
25	ATOM	72	CB	ASP	Y	696	-45.211	87.192	14.322	1.00	40.00	6
	ATOM	73	CG	ASP	Y	696	-44.021	86.560	15.058	1.00	40.00	6
	ATOM	74	OD1	ASP	Y	696	-42.823	86.994	14.844	1.00	40.00	8
	ATOM	75	OD2	ASP	Y	696	-44.212	85.591	15.889	1.00	40.00	8
	END											
30												

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## Appendix 2

Atomic Coordinates for Human ER $\alpha$  Complexed with DES, and a GRIP1 NR-box 2 Peptide

		CRYST1	54.094	82.217	58.041	90.00	111.33	90.00	P	21	2
10	ORIGX1	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000				
	ORIGX2	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000				
	ORIGX3	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000				
	SCALE1	0.018486	0.000000	0.007221	0.000000	0.000000	0.000000				
15	SCALE2	0.000000	0.012163	0.000000	0.000000	0.000000	0.000000				
	SCALE3	0.000000	0.000000	0.018497	0.000000	0.000000	0.000000				
	ATOM	1	CB	SER	A	305	35.230	-14.787	-1.163	1.00	73.26
	ATOM	2	C	SER	A	305	35.331	-14.303	1.289	1.00	72.95
20	ATOM	3	O	SER	A	305	34.146	-13.984	1.186	1.00	72.46
	ATOM	4	N	SER	A	305	36.797	-16.033	0.285	1.00	74.06
	ATOM	5	CA	SER	A	305	36.138	-14.713	0.061	1.00	73.59
	ATOM	6	N	LEU	A	306	35.982	-14.313	2.449	1.00	72.21
	ATOM	7	CA	LEU	A	306	35.329	-13.950	3.702	1.00	71.05
25	ATOM	8	CB	LEU	A	306	36.251	-14.256	4.878	1.00	70.19
	ATOM	9	C	LEU	A	306	34.929	-12.478	3.719	1.00	69.57
	ATOM	10	O	LEU	A	306	35.580	-11.638	3.100	1.00	69.96
	ATOM	11	N	ALA	A	307	33.851	-12.176	4.434	1.00	68.06
	ATOM	12	CA	ALA	A	307	33.358	-10.810	4.541	1.00	64.88
30	ATOM	13	CB	ALA	A	307	31.841	-10.795	4.436	1.00	65.83
	ATOM	14	C	ALA	A	307	33.792	-10.204	5.866	1.00	63.36
	ATOM	15	O	ALA	A	307	33.878	-8.984	6.005	1.00	62.73
	ATOM	16	N	LEU	A	308	34.064	-11.062	6.842	1.00	62.52
	ATOM	17	CA	LEU	A	308	34.487	-10.598	8.156	1.00	62.57
35	ATOM	18	CB	LEU	A	308	34.423	-11.745	9.171	1.00	62.81
	ATOM	19	CG	LEU	A	308	33.214	-12.688	9.130	1.00	64.21
	ATOM	20	CD1	LEU	A	308	33.188	-13.513	10.406	1.00	66.28
	ATOM	21	CD2	LEU	A	308	31.919	-11.898	8.989	1.00	63.80
	ATOM	22	C	LEU	A	308	35.903	-10.037	8.100	1.00	61.61
40	ATOM	23	O	LEU	A	308	36.385	-9.445	9.066	1.00	62.92
	ATOM	24	N	SER	A	309	36.561	-10.219	6.959	1.00	60.50
	ATOM	25	CA	SER	A	309	37.928	-9.743	6.771	1.00	58.73
	ATOM	26	CB	SER	A	309	38.720	-10.750	5.934	1.00	59.53
	ATOM	27	OG	SER	A	309	38.889	-10.283	4.606	1.00	59.47
45	ATOM	28	C	SER	A	309	37.986	-8.373	6.099	1.00	57.05
	ATOM	29	O	SER	A	309	38.965	-7.637	6.249	1.00	56.70
	ATOM	30	N	LEU	A	310	36.940	-8.038	5.352	1.00	52.69
	ATOM	31	CA	LEU	A	310	36.877	-6.759	4.658	1.00	48.20
	ATOM	32	CB	LEU	A	310	35.516	-6.596	3.974	1.00	48.32
50	ATOM	33	CG	LEU	A	310	35.301	-7.188	2.583	1.00	44.94
	ATOM	34	CD1	LEU	A	310	33.951	-6.728	2.055	1.00	46.45
	ATOM	35	CD2	LEU	A	310	36.417	-6.755	1.650	1.00	43.19
	ATOM	36	C	LEU	A	310	37.086	-5.589	5.609	1.00	46.44
	ATOM	37	O	LEU	A	310	36.605	-5.607	6.741	1.00	46.78
55	ATOM	38	N	THR	A	311	37.812	-4.576	5.148	1.00	44.36
	ATOM	39	CA	THR	A	311	38.034	-3.380	5.949	1.00	42.88
	ATOM	40	CB	THR	A	311	39.313	-2.633	5.532	1.00	42.31
	ATOM	41	OG1	THR	A	311	39.079	-1.936	4.303	1.00	42.50
	ATOM	42	CG2	THR	A	311	40.464	-3.606	5.350	1.00	46.02
60	ATOM	43	C	THR	A	311	36.834	-2.475	5.674	1.00	43.21



5	ATOM	44	O	THR	A	311	36.021	-2.776	4.800	1.00	42.12
	ATOM	45	N	ALA	A	312	36.726	-1.372	6.409	1.00	42.16
	ATOM	46	CA	ALA	A	312	35.616	-0.444	6.228	1.00	40.10
	ATOM	47	CB	ALA	A	312	35.741	0.709	7.205	1.00	40.07
	ATOM	48	C	ALA	A	312	35.561	0.090	4.799	1.00	41.80
10	ATOM	49	O	ALA	A	312	34.510	0.074	4.154	1.00	37.81
	ATOM	50	N	ASP	A	313	36.698	0.564	4.304	1.00	42.35
	ATOM	51	CA	ASP	A	313	36.752	1.104	2.953	1.00	42.27
	ATOM	52	CB	ASP	A	313	38.133	1.703	2.680	1.00	43.74
	ATOM	53	CG	ASP	A	313	38.323	3.054	3.348	1.00	46.62
15	ATOM	54	OD1	ASP	A	313	39.414	3.645	3.205	1.00	51.01
	ATOM	55	OD2	ASP	A	313	37.380	3.529	4.015	1.00	48.89
	ATOM	56	C	ASP	A	313	36.422	0.027	1.926	1.00	38.68
	ATOM	57	O	ASP	A	313	35.704	0.281	0.959	1.00	38.75
	ATOM	58	N	GLN	A	314	36.931	-1.179	2.145	1.00	34.76
20	ATOM	59	CA	GLN	A	314	36.666	-2.277	1.229	1.00	33.55
	ATOM	60	CB	GLN	A	314	37.462	-3.512	1.643	1.00	36.90
	ATOM	61	CG	GLN	A	314	38.963	-3.384	1.436	1.00	40.45
	ATOM	62	CD	GLN	A	314	39.700	-4.610	1.905	1.00	43.13
	ATOM	63	OE1	GLN	A	314	39.394	-5.196	2.935	1.00	43.60
25	ATOM	64	NE2	GLN	A	314	40.701	-5.032	1.117	1.00	44.03
	ATOM	65	C	GLN	A	314	35.176	-2.595	1.201	1.00	34.95
	ATOM	66	O	GLN	A	314	34.605	-2.860	0.140	1.00	32.89
	ATOM	67	N	MET	A	315	34.542	-2.564	2.374	1.00	32.54
	ATOM	68	CA	MET	A	315	33.115	-2.848	2.470	1.00	35.46
30	ATOM	69	CB	MET	A	315	32.650	-2.794	3.926	1.00	37.09
	ATOM	70	CG	MET	A	315	31.137	-2.777	4.097	1.00	39.42
	ATOM	71	SD	MET	A	315	30.443	-4.426	4.053	1.00	46.55
	ATOM	72	CE	MET	A	315	31.351	-5.205	5.397	1.00	45.29
	ATOM	73	C	MET	A	315	32.311	-1.859	1.640	1.00	31.83
35	ATOM	74	O	MET	A	315	31.453	-2.247	0.852	1.00	32.10
	ATOM	75	N	VAL	A	316	32.587	-0.560	1.830	1.00	32.62
	ATOM	76	CA	VAL	A	316	31.882	0.470	1.079	1.00	31.09
	ATOM	77	CB	VAL	A	316	32.395	1.888	1.425	1.00	34.77
	ATOM	78	CG1	VAL	A	316	31.786	2.899	0.461	1.00	34.10
40	ATOM	79	CG2	VAL	A	316	32.021	2.246	2.862	1.00	34.40
	ATOM	80	C	VAL	A	316	32.092	0.232	-0.414	1.00	33.48
	ATOM	81	O	VAL	A	316	31.145	0.266	-1.200	1.00	32.49
	ATOM	82	N	SER	A	317	33.337	-0.027	-0.795	1.00	33.49
	ATOM	83	CA	SER	A	317	33.682	-0.280	-2.187	1.00	32.88
45	ATOM	84	CB	SER	A	317	35.165	-0.635	-2.297	1.00	35.77
	ATOM	85	OG	SER	A	317	35.825	0.277	-3.154	1.00	42.70
	ATOM	86	C	SER	A	317	32.849	-1.396	-2.801	1.00	30.71
	ATOM	87	O	SER	A	317	32.279	-1.238	-3.880	1.00	31.14
	ATOM	88	N	ALA	A	318	32.792	-2.529	-2.111	1.00	29.51
50	ATOM	89	CA	ALA	A	318	32.035	-3.676	-2.580	1.00	29.93
	ATOM	90	CB	ALA	A	318	32.156	-4.811	-1.579	1.00	28.56
	ATOM	91	C	ALA	A	318	30.565	-3.305	-2.771	1.00	31.55
	ATOM	92	O	ALA	A	318	29.961	-3.642	-3.784	1.00	30.64
	ATOM	93	N	LEU	A	319	29.997	-2.614	-1.791	1.00	34.13
55	ATOM	94	CA	LEU	A	319	28.597	-2.212	-1.861	1.00	32.93
	ATOM	95	CB	LEU	A	319	28.170	-1.576	-0.540	1.00	31.15
	ATOM	96	CG	LEU	A	319	28.076	-2.555	0.632	1.00	32.27
	ATOM	97	CD1	LEU	A	319	27.523	-1.840	1.852	1.00	32.14
	ATOM	98	CD2	LEU	A	319	27.194	-3.733	0.243	1.00	31.82
60	ATOM	99	C	LEU	A	319	28.340	-1.257	-3.020	1.00	34.41
	ATOM	100	O	LEU	A	319	27.430	-1.475	-3.818	1.00	35.23

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							29.140	-0.195	-3.120	1.00	32.53
5	ATOM	101	N	LEU	A	320	28.972	0.756	-4.212	1.00	35.33
	ATOM	102	CA	LEU	A	320	30.052	1.839	-4.155	1.00	33.52
	ATOM	103	CB	LEU	A	320	29.974	2.899	-3.054	1.00	34.60
	ATOM	104	CG	LEU	A	320	31.060	3.940	-3.292	1.00	33.69
	ATOM	105	CD1	LEU	A	320	28.611	3.562	-3.044	1.00	31.05
10	ATOM	106	CD2	LEU	A	320	29.052	0.040	-5.561	1.00	35.41
	ATOM	107	C	LEU	A	320	28.230	0.271	-6.446	1.00	39.16
	ATOM	108	O	LEU	A	320	30.042	-0.833	-5.720	0.50	36.33
	ATOM	109	N	AASP	A	321	30.041	-0.839	-5.695	0.50	35.76
	ATOM	110	N	BASP	A	321	30.214	-1.559	-6.977	0.50	37.71
15	ATOM	111	CA	AASP	A	321	30.258	-1.595	-6.925	0.50	37.11
	ATOM	112	CA	BASP	A	321	31.537	-2.334	-6.973	0.50	40.01
	ATOM	113	CB	AASP	A	321	31.573	-2.374	-6.826	0.50	39.41
	ATOM	114	CB	BASP	A	321	31.694	-3.230	-8.195	0.50	41.93
	ATOM	115	CG	AASP	A	321	32.770	-1.562	-7.284	0.50	39.96
20	ATOM	116	CG	BASP	A	321	31.523	-2.733	-9.329	0.50	42.11
	ATOM	117	OD1	AASP	A	321	33.312	-1.868	-8.366	0.50	43.41
	ATOM	118	OD1	BASP	A	321	31.988	-4.432	-8.022	0.50	42.69
	ATOM	119	OD2	AASP	A	321	33.170	-0.622	-6.564	0.50	41.33
	ATOM	120	OD2	BASP	A	321	29.069	-2.524	-7.275	0.50	37.19
25	ATOM	121	C	AASP	A	321	29.123	-2.565	-7.253	0.50	36.68
	ATOM	122	C	BASP	A	321	28.820	-2.861	-8.434	0.50	36.87
	ATOM	123	O	AASP	A	321	28.934	-2.942	-8.411	0.50	36.08
	ATOM	124	O	BASP	A	321	28.374	-2.968	-6.235	1.00	35.35
	ATOM	125	N	ALA	A	322	27.268	-3.902	-6.417	1.00	31.59
30	ATOM	126	CA	ALA	A	322	27.124	-4.781	-5.175	1.00	30.73
	ATOM	127	CB	ALA	A	322	25.946	-3.204	-6.709	1.00	30.07
	ATOM	128	C	ALA	A	322	24.955	-3.857	-7.036	1.00	26.53
	ATOM	129	O	ALA	A	322	25.932	-1.880	-6.596	1.00	27.98
	ATOM	130	N	GLU	A	323	24.713	-1.117	-6.827	1.00	29.88
35	ATOM	131	CA	GLU	A	323	25.027	0.380	-6.855	1.00	30.98
	ATOM	132	CB	GLU	A	323	24.870	1.068	-5.509	1.00	31.62
	ATOM	133	CG	GLU	A	323	23.463	0.940	-4.960	1.00	31.98
	ATOM	134	CD	GLU	A	323	23.183	-0.056	-4.257	1.00	33.10
	ATOM	135	OE1	GLU	A	323	22.640	1.836	-5.233	1.00	30.01
40	ATOM	136	OE2	GLU	A	323	24.010	-1.515	-8.123	1.00	30.86
	ATOM	137	C	GLU	A	323	24.655	-1.705	-9.151	1.00	28.86
	ATOM	138	O	GLU	A	323	22.674	-1.659	-8.083	1.00	30.66
	ATOM	139	N	PRO	A	324	21.774	-1.466	-6.935	1.00	31.01
	ATOM	140	CD	PRO	A	324	21.935	-2.032	-9.290	1.00	30.29
45	ATOM	141	CA	PRO	A	324	20.613	-2.598	-8.760	1.00	31.42
	ATOM	142	CB	PRO	A	324	20.626	-2.363	-7.258	1.00	33.66
	ATOM	143	CG	PRO	A	324	21.717	-0.785	-10.138	1.00	27.46
	ATOM	144	C	PRO	A	324	21.893	0.332	-9.668	1.00	26.19
	ATOM	145	O	PRO	A	324	21.335	-0.959	-11.403	1.00	27.80
50	ATOM	146	N	PRO	A	325	21.082	-2.198	-12.161	1.00	27.35
	ATOM	147	CD	PRO	A	325	21.125	0.242	-12.211	1.00	25.59
	ATOM	148	CA	PRO	A	325	21.258	-0.266	-13.637	1.00	24.02
	ATOM	149	CB	PRO	A	325	20.773	-1.695	-13.559	1.00	26.00
	ATOM	150	CG	PRO	A	325	19.749	0.830	-11.954	1.00	23.73
55	ATOM	151	C	PRO	A	325	18.873	0.165	-11.402	1.00	24.83
	ATOM	152	O	PRO	A	325	19.571	2.081	-12.352	1.00	22.11
	ATOM	153	N	ILE	A	326	18.296	2.762	-12.212	1.00	24.01
	ATOM	154	CA	ILE	A	326	18.502	4.282	-12.133	1.00	25.97
	ATOM	155	CB	ILE	A	326	17.168	4.992	-12.286	1.00	20.75
60	ATOM	156	CG2	ILE	A	326	19.189	4.632	-10.805	1.00	29.31
	ATOM	157	CG1	ILE	A	326					

5	ATOM	158	CD1	ILE	A	326	19.301	6.120-10.525	1.00	32.91
	ATOM	159	C	ILE	A	326	17.506	2.408-13.471	1.00	25.72
	ATOM	160	O	ILE	A	326	17.906	2.758-14.581	1.00	25.55
	ATOM	161	N	LEU	A	327	16.392	1.703-13.301	1.00	25.57
	ATOM	162	CA	LEU	A	327	15.595	1.279-14.439	1.00	23.80
10	ATOM	163	CB	LEU	A	327	14.872	-0.029-14.104	1.00	23.96
	ATOM	164	CG	LEU	A	327	15.778	-1.210-13.728	1.00	19.89
	ATOM	165	CD1	LEU	A	327	14.944	-2.462-13.583	1.00	21.19
	ATOM	166	CD2	LEU	A	327	16.850	-1.415-14.805	1.00	17.53
	ATOM	167	C	LEU	A	327	14.598	2.317-14.935	1.00	27.16
15	ATOM	168	O	LEU	A	327	14.161	3.202-14.194	1.00	25.98
	ATOM	169	N	TYR	A	328	14.251	2.207-16.210	1.00	26.56
	ATOM	170	CA	TYR	A	328	13.303	3.123-16.814	1.00	24.45
	ATOM	171	CB	TYR	A	328	13.724	3.465-18.245	1.00	26.72
	ATOM	172	CG	TYR	A	328	14.587	4.693-18.314	1.00	27.73
20	ATOM	173	CD1	TYR	A	328	14.021	5.949-18.518	1.00	28.56
	ATOM	174	CE1	TYR	A	328	14.798	7.092-18.509	1.00	29.10
	ATOM	175	CD2	TYR	A	328	15.962	4.612-18.110	1.00	26.01
	ATOM	176	CE2	TYR	A	328	16.750	5.753-18.098	1.00	30.63
	ATOM	177	CZ	TYR	A	328	16.157	6.988-18.297	1.00	30.07
25	ATOM	178	OH	TYR	A	328	16.917	8.130-18.265	1.00	37.94
	ATOM	179	C	TYR	A	328	11.923	2.501-16.827	1.00	24.95
	ATOM	180	O	TYR	A	328	11.774	1.274-16.846	1.00	27.02
	ATOM	181	N	SER	A	329	10.912	3.358-16.800	1.00	25.60
	ATOM	182	CA	SER	A	329	9.533	2.908-16.837	1.00	29.45
30	ATOM	183	CB	SER	A	329	8.661	3.858-16.020	1.00	30.80
	ATOM	184	OG	SER	A	329	7.297	3.721-16.364	1.00	33.74
	ATOM	185	C	SER	A	329	9.129	2.947-18.313	1.00	31.30
	ATOM	186	O	SER	A	329	9.908	3.397-19.154	1.00	27.35
	ATOM	187	N	GLU	A	330	7.930	2.469-18.629	1.00	32.98
35	ATOM	188	CA	GLU	A	330	7.459	2.482-20.007	1.00	35.10
	ATOM	189	CB	GLU	A	330	6.031	1.968-20.074	1.00	34.67
	ATOM	190	C	GLU	A	330	7.532	3.924-20.505	1.00	40.06
	ATOM	191	O	GLU	A	330	7.068	4.841-19.826	1.00	42.65
	ATOM	192	N	TYR	A	331	8.124	4.126-21.681	1.00	41.16
40	ATOM	193	CA	TYR	A	331	8.263	5.470-22.234	1.00	42.66
	ATOM	194	CB	TYR	A	331	9.323	5.482-23.350	1.00	42.54
	ATOM	195	CG	TYR	A	331	9.202	4.347-24.345	1.00	38.67
	ATOM	196	CD1	TYR	A	331	10.105	3.284-24.334	1.00	34.66
	ATOM	197	CE1	TYR	A	331	9.985	2.228-25.233	1.00	34.89
45	ATOM	198	CD2	TYR	A	331	8.174	4.327-25.287	1.00	37.88
	ATOM	199	CE2	TYR	A	331	8.045	3.276-26.193	1.00	34.65
	ATOM	200	CZ	TYR	A	331	8.950	2.232-26.159	1.00	30.73
	ATOM	201	OH	TYR	A	331	8.814	1.191-27.042	1.00	30.97
	ATOM	202	C	TYR	A	331	6.943	6.043-22.754	1.00	46.24
50	ATOM	203	O	TYR	A	331	6.018	5.301-23.096	1.00	45.38
	ATOM	204	N	ASP	A	332	6.868	7.372-22.792	1.00	49.11
	ATOM	205	CA	ASP	A	332	5.684	8.092-23.262	1.00	52.40
	ATOM	206	CB	ASP	A	332	5.781	8.321-24.772	1.00	52.86
	ATOM	207	C	ASP	A	332	4.356	7.410-22.926	1.00	52.90
55	ATOM	208	O	ASP	A	332	3.561	7.116-23.818	1.00	53.94
	ATOM	209	N	PRO	A	333	4.103	7.144-21.632	1.00	53.63
	ATOM	210	CD	PRO	A	333	4.962	7.418-20.465	1.00	53.63
	ATOM	211	CA	PRO	A	333	2.840	6.497-21.253	1.00	53.55
	ATOM	212	CB	PRO	A	333	3.070	6.076-19.802	1.00	53.78
60	ATOM	213	CG	PRO	A	333	4.101	7.028-19.290	1.00	53.42
	ATOM	214	C	PRO	A	333	1.673	7.478-21.398	1.00	52.17

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5	ATOM	215	O	PRO	A	333	1.879	8.690-21.395	1.00	51.19
	ATOM	216	N	THR	A	334	0.457	6.956-21.532	1.00	52.26
	ATOM	217	CA	THR	A	334	-0.724	7.802-21.687	1.00	54.21
	ATOM	218	CB	THR	A	334	-1.997	6.949-21.813	1.00	53.90
10	ATOM	219	OG1	THR	A	334	-1.971	6.256-23.065	1.00	53.92
	ATOM	220	CG2	THR	A	334	-3.237	7.821-21.761	1.00	54.15
	ATOM	221	C	THR	A	334	-0.864	8.782-20.525	1.00	56.34
	ATOM	222	O	THR	A	334	-1.389	8.443-19.461	1.00	56.44
15	ATOM	223	N	ARG	A	335	-0.386	10.002-20.766	1.00	58.24
	ATOM	224	CA	ARG	A	335	-0.377	11.099-19.801	1.00	57.96
	ATOM	225	CB	ARG	A	335	-0.569	12.427-20.531	1.00	60.22
	ATOM	226	C	ARG	A	335	-1.349	10.996-18.627	1.00	56.61
20	ATOM	227	O	ARG	A	335	-0.919	10.908-17.475	1.00	60.70
	ATOM	228	N	PRO	A	336	-2.667	11.015-18.889	1.00	52.43
	ATOM	229	CD	PRO	A	336	-3.389	11.117-20.165	1.00	49.06
	ATOM	230	CA	PRO	A	336	-3.587	10.915-17.752	1.00	49.58
25	ATOM	231	CB	PRO	A	336	-4.911	11.456-18.302	1.00	48.66
	ATOM	232	CG	PRO	A	336	-4.645	11.809-19.760	1.00	51.33
	ATOM	233	C	PRO	A	336	-3.698	9.468-17.279	1.00	49.25
	ATOM	234	O	PRO	A	336	-4.340	8.644-17.929	1.00	48.06
30	ATOM	235	N	PHE	A	337	-3.063	9.170-16.147	1.00	47.90
	ATOM	236	CA	PHE	A	337	-3.055	7.821-15.582	1.00	46.61
	ATOM	237	CB	PHE	A	337	-2.063	7.732-14.421	1.00	47.73
	ATOM	238	CG	PHE	A	337	-0.649	8.011-14.805	1.00	46.27
35	ATOM	239	CD1	PHE	A	337	-0.017	9.168-14.368	1.00	46.55
	ATOM	240	CD2	PHE	A	337	0.061	7.113-15.591	1.00	48.12
	ATOM	241	CE1	PHE	A	337	1.305	9.429-14.707	1.00	48.09
	ATOM	242	CE2	PHE	A	337	1.386	7.364-15.938	1.00	47.57
40	ATOM	243	CZ	PHE	A	337	2.009	8.525-15.495	1.00	48.40
	ATOM	244	C	PHE	A	337	-4.401	7.338-15.071	1.00	46.15
	ATOM	245	O	PHE	A	337	-5.250	8.127-14.671	1.00	48.34
	ATOM	246	N	SER	A	338	-4.573	6.022-15.080	1.00	45.06
45	ATOM	247	CA	SER	A	338	-5.781	5.385-14.578	1.00	45.12
	ATOM	248	CB	SER	A	338	-6.477	4.594-15.684	1.00	44.49
	ATOM	249	OG	SER	A	338	-6.227	3.206-15.554	1.00	45.78
	ATOM	250	C	SER	A	338	-5.292	4.439-13.488	1.00	47.04
50	ATOM	251	O	SER	A	338	-4.090	4.186-13.387	1.00	44.08
	ATOM	252	N	GLU	A	339	-6.206	3.916-12.676	1.00	45.63
	ATOM	253	CA	GLU	A	339	-5.802	3.012-11.608	1.00	45.40
	ATOM	254	CB	GLU	A	339	-7.015	2.521-10.814	1.00	45.66
55	ATOM	255	CG	GLU	A	339	-6.637	1.680 -9.600	1.00	46.81
	ATOM	256	CD	GLU	A	339	-6.637	1.652 -8.535	1.00	47.56
	ATOM	257	OE1	GLU	A	339	-7.717	0.656 -8.477	1.00	47.37
	ATOM	258	OE2	GLU	A	339	-8.471	2.625 -7.754	1.00	49.29
60	ATOM	259	C	GLU	A	339	-7.810	1.821-12.170	1.00	45.23
	ATOM	260	O	GLU	A	339	-5.040	1.641-11.872	1.00	46.51
	ATOM	261	N	ALA	A	340	-3.862	1.010-12.982	1.00	42.87
	ATOM	262	CA	ALA	A	340	-5.712	-0.158-13.574	1.00	40.24
55	ATOM	263	CB	ALA	A	340	-5.078	-0.871-14.496	1.00	41.40
	ATOM	264	C	ALA	A	340	-6.055	0.273-14.350	1.00	38.83
	ATOM	265	O	ALA	A	340	-3.837	-0.515-14.543	1.00	35.58
	ATOM	266	N	SER	A	341	-2.909	1.535-14.773	1.00	35.79
60	ATOM	267	CA	SER	A	341	-3.836	2.133-15.537	1.00	36.58
	ATOM	268	CB	SER	A	341	-2.742	3.454-16.154	1.00	39.01
	ATOM	269	OG	SER	A	341	-3.231	4.130-16.864	1.00	36.09
	ATOM	270	C	SER	A	341	-2.211	2.376-14.691	1.00	35.63
60	ATOM	271	O	SER	A	341	-1.480	1.913-15.038	1.00	33.20
	ATOM	271	O	SER	A	341	-0.389			

5	ATOM	272	N	MET	A	342	-1.626	3.115-13.595	1.00	35.92
	ATOM	273	CA	MET	A	342	-0.498	3.396-12.708	1.00	35.88
	ATOM	274	CB	MET	A	342	-0.912	4.396-11.623	1.00	35.96
	ATOM	275	CG	MET	A	342	0.241	5.218-11.059	1.00	38.02
	ATOM	276	SD	MET	A	342	-0.308	6.374 -9.780	1.00	44.73
10	ATOM	277	CE	MET	A	342	0.626	7.815-10.205	1.00	42.49
	ATOM	278	C	MET	A	342	-0.011	2.100-12.059	1.00	34.17
	ATOM	279	O	MET	A	342	1.195	1.880-11.909	1.00	33.40
	ATOM	280	N	MET	A	343	-0.957	1.243-11.687	1.00	29.95
	ATOM	281	CA	MET	A	343	-0.640	-0.034-11.062	1.00	31.96
15	ATOM	282	CB	MET	A	343	-1.921	-0.810-10.751	1.00	31.70
	ATOM	283	CG	MET	A	343	-2.667	-0.337 -9.502	1.00	37.13
	ATOM	284	SD	MET	A	343	-1.749	-0.507 -7.940	1.00	36.00
	ATOM	285	CE	MET	A	343	-1.468	-2.299 -7.886	1.00	32.14
	ATOM	286	C	MET	A	343	0.234	-0.875-11.979	1.00	31.72
20	ATOM	287	O	MET	A	343	1.159	-1.558-11.527	1.00	30.26
	ATOM	288	N	GLY	A	344	-0.069	-0.823-13.272	1.00	29.04
	ATOM	289	CA	GLY	A	344	0.688	-1.591-14.242	1.00	24.94
	ATOM	290	C	GLY	A	344	2.104	-1.085-14.396	1.00	26.01
	ATOM	291	O	GLY	A	344	3.046	-1.873-14.463	1.00	28.72
25	ATOM	292	N	LEU	A	345	2.257	0.232-14.471	1.00	26.97
	ATOM	293	CA	LEU	A	345	3.576	0.839-14.608	1.00	31.15
	ATOM	294	CB	LEU	A	345	3.459	2.361-14.753	1.00	30.06
	ATOM	295	CG	LEU	A	345	2.765	2.924-15.995	1.00	33.50
	ATOM	296	CD1	LEU	A	345	2.901	4.439-15.999	1.00	33.52
30	ATOM	297	CD2	LEU	A	345	3.379	2.324-17.257	1.00	33.22
	ATOM	298	C	LEU	A	345	4.433	0.534-13.383	1.00	30.31
	ATOM	299	O	LEU	A	345	5.564	0.061-13.505	1.00	32.80
	ATOM	300	N	LEU	A	346	3.884	0.813-12.205	1.00	27.83
	ATOM	301	CA	LEU	A	346	4.595	0.596-10.947	1.00	26.19
35	ATOM	302	CB	LEU	A	346	3.729	1.063 -9.783	1.00	24.51
	ATOM	303	CG	LEU	A	346	3.483	2.569 -9.682	1.00	26.33
	ATOM	304	CD1	LEU	A	346	2.623	2.844 -8.463	1.00	27.33
	ATOM	305	CD2	LEU	A	346	4.809	3.317 -9.587	1.00	24.89
	ATOM	306	C	LEU	A	346	5.032	-0.848-10.707	1.00	25.72
40	ATOM	307	O	LEU	A	346	6.181	-1.102-10.345	1.00	29.86
	ATOM	308	N	THR	A	347	4.117	-1.793-10.891	1.00	23.80
	ATOM	309	CA	THR	A	347	4.436	-3.196-10.674	1.00	23.91
	ATOM	310	CB	THR	A	347	3.164	-4.058-10.641	1.00	26.39
	ATOM	311	OG1	THR	A	347	2.421	-3.860-11.849	1.00	24.57
45	ATOM	312	CG2	THR	A	347	2.301	-3.682 -9.444	1.00	23.98
	ATOM	313	C	THR	A	347	5.366	-3.734-11.756	1.00	26.17
	ATOM	314	O	THR	A	347	6.176	-4.622-11.496	1.00	27.44
	ATOM	315	N	ASN	A	348	5.242	-3.197-12.970	1.00	25.48
	ATOM	316	CA	ASN	A	348	6.092	-3.617-14.082	1.00	23.77
50	ATOM	317	CB	ASN	A	348	5.657	-2.926-15.385	1.00	24.59
	ATOM	318	CG	ASN	A	348	6.522	-3.302-16.571	1.00	29.93
	ATOM	319	OD1	ASN	A	348	7.616	-2.799-16.771	1.00	24.81
	ATOM	320	ND2	ASN	A	348	6.010	-4.236-17.391	1.00	32.61
	ATOM	321	C	ASN	A	348	7.532	-3.229-13.741	1.00	22.82
55	ATOM	322	O	ASN	A	348	8.453	-4.027-13.870	1.00	18.83
	ATOM	323	N	LEU	A	349	7.711	-1.993-13.288	1.00	22.58
	ATOM	324	CA	LEU	A	349	9.030	-1.507-12.914	1.00	21.85
	ATOM	325	CB	LEU	A	349	8.929	-0.028-12.536	1.00	22.00
	ATOM	326	CG	LEU	A	349	10.155	0.673-11.953	1.00	23.64
60	ATOM	327	CD1	LEU	A	349	11.224	0.826-13.017	1.00	19.35
	ATOM	328	CD2	LEU	A	349	9.726	2.040-11.415	1.00	21.97

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5	ATOM	329	C	LEU	A	349	9.564	-2.335-11.734	1.00	22.94
	ATOM	330	O	LEU	A	349	10.724	-2.749-11.717	1.00	23.97
	ATOM	331	N	ALA	A	350	8.705	-2.591-10.756	1.00	21.67
	ATOM	332	CA	ALA	A	350	9.113	-3.356 -9.586	1.00	21.83
10	ATOM	333	CB	ALA	A	350	7.963	-3.441 -8.593	1.00	18.95
	ATOM	334	C	ALA	A	350	9.568	-4.757 -9.985	1.00	21.90
	ATOM	335	O	ALA	A	350	10.625	-5.221 -9.554	1.00	24.15
	ATOM	336	N	ASP	A	351	8.767	-5.423-10.810	1.00	23.24
15	ATOM	337	CA	ASP	A	351	9.093	-6.772-11.259	1.00	25.87
	ATOM	338	CB	ASP	A	351	8.028	-7.274-12.239	1.00	27.03
	ATOM	339	CG	ASP	A	351	8.103	-8.772-12.458	1.00	31.64
	ATOM	340	OD1	ASP	A	351	8.217	-9.196-13.628	1.00	35.06
20	ATOM	341	OD2	ASP	A	351	8.049	-9.525-11.464	1.00	36.86
	ATOM	342	C	ASP	A	351	10.469	-6.825-11.912	1.00	22.36
	ATOM	343	O	ASP	A	351	11.219	-7.773-11.702	1.00	25.15
	ATOM	344	N	ARG	A	352	10.810	-5.808-12.697	1.00	23.58
25	ATOM	345	CA	ARG	A	352	12.115	-5.787-13.347	1.00	21.07
	ATOM	346	CB	ARG	A	352	12.120	-4.785-14.507	1.00	21.02
	ATOM	347	CG	ARG	A	352	11.539	-5.352-15.797	1.00	20.44
	ATOM	348	CD	ARG	A	352	11.554	-4.319-16.915	1.00	20.43
30	ATOM	349	NE	ARG	A	352	10.592	-3.245-16.687	1.00	19.85
	ATOM	350	CZ	ARG	A	352	10.910	-1.954-16.641	1.00	19.69
	ATOM	351	NH1	ARG	A	352	10.910	-1.564-16.813	1.00	17.36
	ATOM	352	NH2	ARG	A	352	12.172	-1.049-16.441	1.00	21.88
35	ATOM	353	C	ARG	A	352	9.962	-5.442-12.350	1.00	22.11
	ATOM	354	O	ARG	A	352	13.223	-5.442-12.350	1.00	22.11
	ATOM	355	N	GLU	A	353	14.346	-5.945-12.454	1.00	24.13
	ATOM	356	CA	GLU	A	353	12.909	-4.587-11.383	1.00	18.66
40	ATOM	357	CB	GLU	A	353	13.888	-4.206-10.376	1.00	19.08
	ATOM	358	CG	GLU	A	353	13.317	-3.102 -9.483	1.00	21.62
	ATOM	359	CD	GLU	A	353	13.295	-1.718-10.114	1.00	20.97
	ATOM	360	OE1	GLU	A	353	12.832	-0.648 -9.129	1.00	23.84
45	ATOM	361	OE2	GLU	A	353	11.611	-0.531 -8.926	1.00	24.76
	ATOM	362	C	GLU	A	353	13.686	0.066 -8.557	1.00	24.95
	ATOM	363	O	GLU	A	353	14.246	-5.423 -9.512	1.00	20.14
	ATOM	364	N	LEU	A	354	15.398	-5.600 -9.104	1.00	19.40
50	ATOM	365	CA	LEU	A	354	13.246	-6.257 -9.235	1.00	19.54
	ATOM	366	CB	LEU	A	354	13.434	-7.452 -8.415	1.00	21.77
	ATOM	367	CG	LEU	A	354	12.107	-8.209 -8.270	1.00	23.09
	ATOM	368	CD1	LEU	A	354	11.160	-7.606 -7.223	1.00	25.00
55	ATOM	369	CD2	LEU	A	354	9.720	-8.013 -7.510	1.00	23.49
	ATOM	370	C	LEU	A	354	11.584	-8.069 -5.839	1.00	23.31
	ATOM	371	O	LEU	A	354	14.500	-8.386 -8.981	1.00	23.21
	ATOM	372	N	VAL	A	355	15.255	-9.007 -8.234	1.00	22.44
60	ATOM	373	CA	VAL	A	355	14.560	-8.490-10.302	1.00	22.52
	ATOM	374	CB	VAL	A	355	15.551	-9.343-10.935	1.00	21.66
	ATOM	375	CG1	VAL	A	355	15.353	-9.365-12.466	1.00	24.35
	ATOM	376	CG2	VAL	A	355	16.435	-10.214-13.119	1.00	28.16
65	ATOM	377	C	VAL	A	355	13.957	-9.886-12.798	1.00	21.59
	ATOM	378	O	VAL	A	355	16.944	-8.811-10.606	1.00	23.74
	ATOM	379	N	HIS	A	356	17.857	-9.581-10.291	1.00	23.51
	ATOM	380	CA	HIS	A	356	17.105	-7.489-10.669	1.00	21.27
70	ATOM	381	CB	HIS	A	356	18.392	-6.861-10.369	1.00	21.31
	ATOM	382	CG	HIS	A	356	18.384	-5.390-10.811	1.00	19.87
	ATOM	383	CD2	HIS	A	356	18.494	-5.205-12.295	1.00	21.77
	ATOM	384	ND1	HIS	A	356	17.543	-5.048-13.248	1.00	21.66
75	ATOM	385	CE1	HIS	A	356	19.704	-5.177-12.955	1.00	21.11
	ATOM	385	CE1	HIS	A	356	19.496	-5.011-14.249	1.00	24.96

5	ATOM	386	NE2	HIS	A	356	18.192	-4.931	-14.455	1.00	18.37
	ATOM	387	C	HIS	A	356	18.702	-6.947	-8.875	1.00	21.41
	ATOM	388	O	HIS	A	356	19.864	-7.111	-8.465	1.00	21.88
	ATOM	389	N	MET	A	357	17.660	-6.843	-8.058	1.00	21.84
	ATOM	390	CA	MET	A	357	17.837	-6.906	-6.610	1.00	21.51
10	ATOM	391	CB	MET	A	357	16.503	-6.668	-5.898	1.00	17.60
	ATOM	392	CG	MET	A	357	16.629	-6.579	-4.369	1.00	19.36
	ATOM	393	SD	MET	A	357	15.051	-6.755	-3.531	1.00	23.64
	ATOM	394	CE	MET	A	357	14.189	-5.332	-4.163	1.00	23.13
	ATOM	395	C	MET	A	357	18.411	-8.259	-6.192	1.00	23.69
15	ATOM	396	O	MET	A	357	19.337	-8.328	-5.389	1.00	24.41
	ATOM	397	N	ILE	A	358	17.856	-9.331	-6.746	1.00	27.14
	ATOM	398	CA	ILE	A	358	18.314	-10.672	-6.425	1.00	28.79
	ATOM	399	CB	ILE	A	358	17.529	-11.725	-7.232	1.00	32.42
	ATOM	400	CG2	ILE	A	358	18.267	-13.064	-7.220	1.00	32.77
20	ATOM	401	CG1	ILE	A	358	16.125	-11.880	-6.644	1.00	31.94
	ATOM	402	CD1	ILE	A	358	15.062	-12.196	-7.680	1.00	34.85
	ATOM	403	C	ILE	A	358	19.801	-10.802	-6.728	1.00	28.75
	ATOM	404	O	ILE	A	358	20.569	-11.305	-5.912	1.00	31.60
	ATOM	405	N	ASN	A	359	20.207	-10.325	-7.897	1.00	27.91
25	ATOM	406	CA	ASN	A	359	21.601	-10.401	-8.293	1.00	29.16
	ATOM	407	CB	ASN	A	359	21.721	-10.172	-9.801	1.00	31.88
	ATOM	408	CG	ASN	A	359	21.253	-11.381	-10.599	1.00	39.34
	ATOM	409	OD1	ASN	A	359	21.916	-12.422	-10.612	1.00	41.27
	ATOM	410	ND2	ASN	A	359	20.102	-11.255	-11.253	1.00	38.58
30	ATOM	411	C	ASN	A	359	22.476	-9.436	-7.510	1.00	30.75
	ATOM	412	O	ASN	A	359	23.686	-9.629	-7.412	1.00	33.35
	ATOM	413	N	TRP	A	360	21.872	-8.400	-6.940	1.00	30.07
	ATOM	414	CA	TRP	A	360	22.634	-7.451	-6.132	1.00	27.87
	ATOM	415	CB	TRP	A	360	21.849	-6.150	-5.948	1.00	24.80
35	ATOM	416	CG	TRP	A	360	22.196	-5.392	-4.691	1.00	23.04
	ATOM	417	CD2	TRP	A	360	21.501	-5.443	-3.438	1.00	19.83
	ATOM	418	CE2	TRP	A	360	22.147	-4.543	-2.564	1.00	22.31
	ATOM	419	CE3	TRP	A	360	20.392	-6.165	-2.972	1.00	20.09
	ATOM	420	CD1	TRP	A	360	23.212	-4.488	-4.529	1.00	18.99
40	ATOM	421	NE1	TRP	A	360	23.187	-3.974	-3.255	1.00	21.17
	ATOM	422	CZ2	TRP	A	360	21.721	-4.340	-1.243	1.00	20.43
	ATOM	423	CZ3	TRP	A	360	19.968	-5.965	-1.661	1.00	20.12
	ATOM	424	CH2	TRP	A	360	20.635	-5.057	-0.812	1.00	18.54
	ATOM	425	C	TRP	A	360	22.892	-8.099	-4.766	1.00	24.88
45	ATOM	426	O	TRP	A	360	23.978	-7.980	-4.198	1.00	25.00
	ATOM	427	N	ALA	A	361	21.879	-8.789	-4.252	1.00	24.08
	ATOM	428	CA	ALA	A	361	21.972	-9.462	-2.958	1.00	26.06
	ATOM	429	CB	ALA	A	361	20.676	-10.203	-2.672	1.00	20.27
	ATOM	430	C	ALA	A	361	23.161	-10.433	-2.897	1.00	28.44
50	ATOM	431	O	ALA	A	361	23.843	-10.531	-1.876	1.00	28.95
	ATOM	432	N	LYS	A	362	23.414	-11.144	-3.992	1.00	31.41
	ATOM	433	CA	LYS	A	362	24.530	-12.097	-4.047	1.00	33.33
	ATOM	434	CB	LYS	A	362	24.564	-12.824	-5.390	1.00	34.81
	ATOM	435	CG	LYS	A	362	23.319	-13.608	-5.756	1.00	36.27
55	ATOM	436	CD	LYS	A	362	23.458	-14.178	-7.167	1.00	38.30
	ATOM	437	CE	LYS	A	362	22.369	-15.193	-7.472	1.00	40.94
	ATOM	438	NZ	LYS	A	362	22.111	-15.322	-8.937	1.00	42.49
	ATOM	439	C	LYS	A	362	25.854	-11.351	-3.893	1.00	34.17
	ATOM	440	O	LYS	A	362	26.880	-11.977	-3.595	1.00	35.40
60	ATOM	441	N	AARG	A	363	25.826	-10.059	-4.095	0.50	34.23
	ATOM	442	N	BARG	A	363	25.826	-10.059	-4.095	0.50	34.03

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5	ATOM	443	CA	AARG	A	363	27.035	-9.254	-3.987	0.50	33.25
	ATOM	444	CA	BARG	A	363	27.035	-9.254	-3.987	0.50	32.83
	ATOM	445	CB	AARG	A	363	27.031	-8.153	-5.044	0.50	34.67
	ATOM	446	CB	BARG	A	363	27.031	-8.153	-5.045	0.50	34.20
	ATOM	447	CG	AARG	A	363	26.933	-8.654	-6.478	0.50	36.32
10	ATOM	448	CG	BARG	A	363	26.930	-8.654	-6.480	0.50	35.56
	ATOM	449	CD	AARG	A	363	27.745	-7.775	-7.415	0.50	38.39
	ATOM	450	CD	BARG	A	363	27.752	-7.781	-7.414	0.50	37.18
	ATOM	451	NE	AARG	A	363	29.171	-7.793	-7.091	0.50	39.98
	ATOM	452	NE	BARG	A	363	27.195	-7.725	-8.762	0.50	37.39
15	ATOM	453	CZ	AARG	A	363	30.086	-7.038	-7.692	0.50	40.54
	ATOM	454	CZ	BARG	A	363	27.905	-7.457	-9.855	0.50	40.02
	ATOM	455	NH1	AARG	A	363	29.735	-6.218	-8.675	0.50	38.13
	ATOM	456	NH1	BARG	A	363	29.205	-7.191	-9.761	0.50	40.42
	ATOM	457	NH2	AARG	A	363	31.358	-7.123	-7.326	0.50	43.19
20	ATOM	458	NH2	BARG	A	363	27.311	-7.436	-11.041	0.50	38.91
	ATOM	459	C	AARG	A	363	27.207	-8.630	-2.610	0.50	33.28
	ATOM	460	C	BARG	A	363	27.207	-8.630	-2.610	0.50	32.81
	ATOM	461	O	AARG	A	363	28.223	-7.992	-2.344	0.50	34.18
	ATOM	462	O	BARG	A	363	28.223	-7.992	-2.345	0.50	33.43
25	ATOM	463	N	VAL	A	364	26.215	-8.798	-1.740	1.00	33.12
	ATOM	464	CA	VAL	A	364	26.288	-8.240	-0.389	1.00	33.63
	ATOM	465	CB	VAL	A	364	24.898	-8.178	0.292	1.00	34.97
	ATOM	466	CG1	VAL	A	364	25.036	-7.608	1.700	1.00	35.44
	ATOM	467	CG2	VAL	A	364	23.946	-7.328	-0.532	1.00	36.69
30	ATOM	468	C	VAL	A	364	27.184	-9.157	0.428	1.00	34.27
	ATOM	469	O	VAL	A	364	26.878	-10.341	0.603	1.00	34.95
	ATOM	470	N	PRO	A	365	28.306	-8.626	0.935	1.00	36.08
	ATOM	471	CD	PRO	A	365	28.775	-7.235	0.793	1.00	34.84
	ATOM	472	CA	PRO	A	365	29.231	-9.442	1.733	1.00	37.82
35	ATOM	473	CB	PRO	A	365	30.110	-8.408	2.430	1.00	34.31
	ATOM	474	CG	PRO	A	365	30.127	-7.247	1.475	1.00	37.77
	ATOM	475	C	PRO	A	365	28.538	-10.373	2.720	1.00	37.61
	ATOM	476	O	PRO	A	365	27.692	-9.945	3.507	1.00	37.74
	ATOM	477	N	GLY	A	366	28.890	-11.654	2.654	1.00	39.04
40	ATOM	478	CA	GLY	A	366	28.307	-12.635	3.554	1.00	38.27
	ATOM	479	C	GLY	A	366	26.991	-13.264	3.138	1.00	39.32
	ATOM	480	O	GLY	A	366	26.638	-14.336	3.635	1.00	39.53
	ATOM	481	N	PHE	A	367	26.246	-12.615	2.236	1.00	38.60
	ATOM	482	CA	PHE	A	367	24.960	-13.148	1.783	1.00	36.36
45	ATOM	483	CB	PHE	A	367	24.281	-12.178	0.808	1.00	32.10
	ATOM	484	CG	PHE	A	367	22.827	-12.473	0.581	1.00	30.12
	ATOM	485	CD1	PHE	A	367	22.401	-13.083	-0.596	1.00	28.95
	ATOM	486	CD2	PHE	A	367	21.882	-12.176	1.563	1.00	26.18
	ATOM	487	CE1	PHE	A	367	21.050	-13.400	-0.792	1.00	29.42
50	ATOM	488	CE2	PHE	A	367	20.535	-12.491	1.373	1.00	27.60
	ATOM	489	CZ	PHE	A	367	20.118	-13.103	0.196	1.00	26.81
	ATOM	490	C	PHE	A	367	25.072	-14.519	1.117	1.00	36.82
	ATOM	491	O	PHE	A	367	24.244	-15.398	1.359	1.00	36.55
	ATOM	492	N	VAL	A	368	26.088	-14.694	0.276	1.00	38.28
55	ATOM	493	CA	VAL	A	368	26.289	-15.965	-0.420	1.00	42.34
	ATOM	494	CB	VAL	A	368	27.386	-15.850	-1.504	1.00	41.78
	ATOM	495	CG1	VAL	A	368	26.972	-14.831	-2.550	1.00	44.60
	ATOM	496	CG2	VAL	A	368	28.707	-15.457	-0.873	1.00	42.23
	ATOM	497	C	VAL	A	368	26.664	-17.100	0.533	1.00	43.85
60	ATOM	498	O	VAL	A	368	26.469	-18.274	0.216	1.00	44.85
	ATOM	499	N	ASP	A	369	27.199	-16.750	1.699	1.00	44.93



5	ATOM	500	CA	ASP	A	369	27.579	-17.755	2.688	1.00	44.96
	ATOM	501	CB	ASP	A	369	28.336	-17.106	3.849	1.00	43.76
	ATOM	502	CG	ASP	A	369	29.608	-16.413	3.404	1.00	43.04
	ATOM	503	OD1	ASP	A	369	30.121	-15.570	4.167	1.00	44.32
	ATOM	504	OD2	ASP	A	369	30.097	-16.709	2.293	1.00	46.76
10	ATOM	505	C	ASP	A	369	26.340	-18.465	3.228	1.00	45.89
	ATOM	506	O	ASP	A	369	26.360	-19.671	3.475	1.00	48.61
	ATOM	507	N	LEU	A	370	25.261	-17.714	3.407	1.00	43.59
	ATOM	508	CA	LEU	A	370	24.020	-18.279	3.924	1.00	44.24
	ATOM	509	CB	LEU	A	370	22.980	-17.173	4.110	1.00	41.42
15	ATOM	510	CG	LEU	A	370	23.404	-16.015	5.014	1.00	41.45
	ATOM	511	CD1	LEU	A	370	22.219	-15.095	5.245	1.00	42.25
	ATOM	512	CD2	LEU	A	370	23.931	-16.552	6.332	1.00	38.35
	ATOM	513	C	LEU	A	370	23.449	-19.360	3.013	1.00	44.03
	ATOM	514	O	LEU	A	370	23.773	-19.423	1.829	1.00	43.63
20	ATOM	515	N	THR	A	371	22.593	-20.206	3.575	1.00	44.29
	ATOM	516	CA	THR	A	371	21.968	-21.272	2.806	1.00	44.84
	ATOM	517	CB	THR	A	371	21.293	-22.302	3.730	1.00	45.65
	ATOM	518	OG1	THR	A	371	20.262	-21.663	4.495	1.00	46.43
	ATOM	519	CG2	THR	A	371	22.314	-22.903	4.677	1.00	46.48
25	ATOM	520	C	THR	A	371	20.923	-20.684	1.864	1.00	44.93
	ATOM	521	O	THR	A	371	20.418	-19.585	2.092	1.00	44.36
	ATOM	522	N	LEU	A	372	20.607	-21.418	0.804	1.00	43.83
	ATOM	523	CA	LEU	A	372	19.624	-20.971	-0.166	1.00	44.62
	ATOM	524	CB	LEU	A	372	19.407	-22.043	-1.237	1.00	47.17
30	ATOM	525	CG	LEU	A	372	18.512	-21.690	-2.429	1.00	46.91
	ATOM	526	CD1	LEU	A	372	19.005	-20.417	-3.098	1.00	48.73
	ATOM	527	CD2	LEU	A	372	18.521	-22.844	-3.420	1.00	51.12
	ATOM	528	C	LEU	A	372	18.307	-20.644	0.512	1.00	44.84
	ATOM	529	O	LEU	A	372	17.705	-19.602	0.261	1.00	43.25
35	ATOM	530	N	HIS	A	373	17.849	-21.558	1.382	1.00	43.14
	ATOM	531	CA	HIS	A	373	16.599	-21.353	2.100	1.00	42.23
	ATOM	532	CB	HIS	A	373	16.318	-22.525	3.062	1.00	45.38
	ATOM	533	CG	HIS	A	373	15.114	-22.315	3.934	1.00	51.43
	ATOM	534	CD2	HIS	A	373	13.808	-22.621	3.743	1.00	54.99
40	ATOM	535	ND1	HIS	A	373	15.187	-21.716	5.174	1.00	54.26
	ATOM	536	CE1	HIS	A	373	13.979	-21.663	5.709	1.00	53.77
	ATOM	537	NE2	HIS	A	373	13.124	-22.206	4.861	1.00	55.27
	ATOM	538	C	HIS	A	373	16.665	-20.047	2.885	1.00	39.78
	ATOM	539	O	HIS	A	373	15.677	-19.324	2.971	1.00	37.71
45	ATOM	540	N	ASP	A	374	17.839	-19.738	3.440	1.00	36.38
	ATOM	541	CA	ASP	A	374	18.020	-18.516	4.219	1.00	37.21
	ATOM	542	CB	ASP	A	374	19.287	-18.620	5.073	1.00	38.17
	ATOM	543	CG	ASP	A	374	19.064	-19.425	6.344	1.00	41.47
	ATOM	544	OD1	ASP	A	374	17.896	-19.543	6.772	1.00	37.09
50	ATOM	545	OD2	ASP	A	374	20.052	-19.940	6.912	1.00	44.40
	ATOM	546	C	ASP	A	374	18.083	-17.277	3.326	1.00	37.19
	ATOM	547	O	ASP	A	374	17.598	-16.208	3.696	1.00	38.13
	ATOM	548	N	GLN	A	375	18.688	-17.431	2.152	1.00	33.13
	ATOM	549	CA	GLN	A	375	18.788	-16.339	1.198	1.00	31.94
55	ATOM	550	CB	GLN	A	375	19.634	-16.756	-0.001	1.00	28.81
	ATOM	551	CG	GLN	A	375	21.125	-16.570	0.189	1.00	31.71
	ATOM	552	CD	GLN	A	375	21.920	-17.222	-0.922	1.00	34.49
	ATOM	553	OE1	GLN	A	375	21.478	-17.267	-2.067	1.00	36.09
	ATOM	554	NE2	GLN	A	375	23.097	-17.736	-0.588	1.00	40.32
60	ATOM	555	C	GLN	A	375	17.379	-16.009	0.730	1.00	31.50
	ATOM	556	O	GLN	A	375	16.990	-14.840	0.653	1.00	27.42

5	ATOM	557	N	VAL	A	376	16.617	-17.056	0.429	1.00	30.38
	ATOM	558	CA	VAL	A	376	15.242	-16.907	-0.027	1.00	33.50
	ATOM	559	CB	VAL	A	376	14.588	-18.286	-0.286	1.00	30.57
	ATOM	560	CG1	VAL	A	376	13.093	-18.122	-0.516	1.00	33.14
	ATOM	561	CG2	VAL	A	376	15.232	-18.952	-1.485	1.00	30.79
10	ATOM	562	C	VAL	A	376	14.393	-16.159	1.002	1.00	33.80
	ATOM	563	O	VAL	A	376	13.653	-15.237	0.661	1.00	34.89
	ATOM	564	N	HIS	A	377	14.500	-16.568	2.261	1.00	33.35
	ATOM	565	CA	HIS	A	377	13.730	-15.941	3.329	1.00	32.81
	ATOM	566	CB	HIS	A	377	13.966	-16.694	4.644	1.00	35.24
15	ATOM	567	CG	HIS	A	377	13.429	-15.989	5.851	1.00	40.15
	ATOM	568	CD2	HIS	A	377	14.054	-15.495	6.946	1.00	40.86
	ATOM	569	ND1	HIS	A	377	12.090	-15.703	6.012	1.00	43.08
	ATOM	570	CE1	HIS	A	377	11.913	-15.062	7.154	1.00	42.44
	ATOM	571	NE2	HIS	A	377	13.089	-14.922	7.740	1.00	44.85
20	ATOM	572	C	HIS	A	377	14.058	-14.454	3.507	1.00	28.63
	ATOM	573	O	HIS	A	377	13.158	-13.619	3.613	1.00	29.20
	ATOM	574	N	LEU	A	378	15.343	-14.125	3.544	1.00	24.41
	ATOM	575	CA	LEU	A	378	15.759	-12.738	3.721	1.00	23.21
	ATOM	576	CB	LEU	A	378	17.289	-12.650	3.743	1.00	20.98
25	ATOM	577	CG	LEU	A	378	17.960	-13.190	5.016	1.00	24.22
	ATOM	578	CD1	LEU	A	378	19.471	-13.041	4.924	1.00	21.07
	ATOM	579	CD2	LEU	A	378	17.431	-12.446	6.221	1.00	20.24
	ATOM	580	C	LEU	A	378	15.190	-11.827	2.630	1.00	24.78
	ATOM	581	O	LEU	A	378	14.638	-10.766	2.922	1.00	22.09
30	ATOM	582	N	LEU	A	379	15.321	-12.242	1.374	1.00	24.13
	ATOM	583	CA	LEU	A	379	14.812	-11.447	0.262	1.00	25.02
	ATOM	584	CB	LEU	A	379	15.307	-12.025	-1.062	1.00	27.12
	ATOM	585	CG	LEU	A	379	16.724	-11.600	-1.437	1.00	24.39
	ATOM	586	CD1	LEU	A	379	17.299	-12.557	-2.470	1.00	27.58
35	ATOM	587	CD2	LEU	A	379	16.679	-10.178	-1.983	1.00	29.05
	ATOM	588	C	LEU	A	379	13.287	-11.355	0.246	1.00	27.61
	ATOM	589	O	LEU	A	379	12.726	-10.301	-0.062	1.00	26.16
	ATOM	590	N	GLU	A	380	12.616	-12.454	0.576	1.00	25.65
	ATOM	591	CA	GLU	A	380	11.154	-12.471	0.592	1.00	26.85
40	ATOM	592	CB	GLU	A	380	10.640	-13.882	0.871	1.00	29.38
	ATOM	593	CG	GLU	A	380	10.718	-14.796	-0.331	1.00	35.58
	ATOM	594	CD	GLU	A	380	10.228	-16.194	-0.025	1.00	39.31
	ATOM	595	OE1	GLU	A	380	10.142	-17.008	-0.967	1.00	42.89
	ATOM	596	OE2	GLU	A	380	9.927	-16.478	1.153	1.00	39.45
45	ATOM	597	C	GLU	A	380	10.604	-11.526	1.649	1.00	25.43
	ATOM	598	O	GLU	A	380	9.551	-10.925	1.469	1.00	27.75
	ATOM	599	N	CYS	A	381	11.324	-11.400	2.753	1.00	25.57
	ATOM	600	CA	CYS	A	381	10.907	-10.530	3.843	1.00	26.46
	ATOM	601	CB	CYS	A	381	11.570	-11.000	5.149	1.00	31.46
50	ATOM	602	SG	CYS	A	381	11.305	-9.946	6.623	1.00	45.32
	ATOM	603	C	CYS	A	381	11.262	-9.059	3.589	1.00	24.77
	ATOM	604	O	CYS	A	381	10.516	-8.166	3.975	1.00	25.01
	ATOM	605	N	ALA	A	382	12.377	-8.815	2.903	1.00	22.23
	ATOM	606	CA	ALA	A	382	12.855	-7.449	2.681	1.00	21.83
55	ATOM	607	CB	ALA	A	382	14.319	-7.383	3.095	1.00	21.56
	ATOM	608	C	ALA	A	382	12.705	-6.778	1.311	1.00	19.78
	ATOM	609	O	ALA	A	382	12.996	-5.587	1.182	1.00	17.01
	ATOM	610	N	TRP	A	383	12.261	-7.507	0.294	1.00	17.61
	ATOM	611	CA	TRP	A	383	12.164	-6.915	-1.036	1.00	18.06
60	ATOM	612	CB	TRP	A	383	11.580	-7.928	-2.035	1.00	20.28
	ATOM	613	CG	TRP	A	383	10.105	-8.201	-1.919	1.00	20.50

5	ATOM	614	CD2	TRP	A	383	9.049	-7.509	-2.599	1.00	22.48
	ATOM	615	CE2	TRP	A	383	7.836	-8.138	-2.238	1.00	20.41
	ATOM	616	CE3	TRP	A	383	9.012	-6.420	-3.482	1.00	22.06
	ATOM	617	CD1	TRP	A	383	9.506	-9.189	-1.190	1.00	23.38
	ATOM	618	NE1	TRP	A	383	8.142	-9.159	-1.377	1.00	22.59
10	ATOM	619	CZ2	TRP	A	383	6.598	-7.713	-2.724	1.00	21.98
	ATOM	620	CZ3	TRP	A	383	7.780	-5.998	-3.968	1.00	25.50
	ATOM	621	CH2	TRP	A	383	6.589	-6.647	-3.587	1.00	23.11
	ATOM	622	C	TRP	A	383	11.448	-5.564	-1.170	1.00	19.18
	ATOM	623	O	TRP	A	383	11.972	-4.663	-1.824	1.00	19.27
15	ATOM	624	N	LEU	A	384	10.273	-5.396	-0.567	1.00	18.32
	ATOM	625	CA	LEU	A	384	9.586	-4.118	-0.719	1.00	16.38
	ATOM	626	CB	LEU	A	384	8.125	-4.218	-0.258	1.00	16.79
	ATOM	627	CG	LEU	A	384	7.211	-3.013	-0.577	1.00	18.39
	ATOM	628	CD1	LEU	A	384	7.464	-2.485	-1.995	1.00	13.91
20	ATOM	629	CD2	LEU	A	384	5.750	-3.432	-0.410	1.00	18.38
	ATOM	630	C	LEU	A	384	10.324	-3.027	0.051	1.00	18.80
	ATOM	631	O	LEU	A	384	10.334	-1.870	-0.357	1.00	20.90
	ATOM	632	N	GLU	A	385	10.949	-3.404	1.163	1.00	18.61
	ATOM	633	CA	GLU	A	385	11.718	-2.462	1.970	1.00	19.58
25	ATOM	634	CB	GLU	A	385	12.274	-3.154	3.213	1.00	17.43
	ATOM	635	CG	GLU	A	385	11.292	-3.237	4.357	1.00	22.92
	ATOM	636	CD	GLU	A	385	11.963	-3.676	5.640	1.00	25.83
	ATOM	637	OE1	GLU	A	385	12.431	-2.799	6.391	1.00	23.69
	ATOM	638	OE2	GLU	A	385	12.027	-4.897	5.889	1.00	27.64
30	ATOM	639	C	GLU	A	385	12.890	-1.934	1.156	1.00	19.46
	ATOM	640	O	GLU	A	385	13.206	-0.743	1.196	1.00	15.04
	ATOM	641	N	ILE	A	386	13.539	-2.842	0.431	1.00	13.32
	ATOM	642	CA	ILE	A	386	14.685	-2.484	-0.388	1.00	15.01
	ATOM	643	CB	ILE	A	386	15.475	-3.763	-0.807	1.00	17.43
35	ATOM	644	CG2	ILE	A	386	16.544	-3.424	-1.849	1.00	17.99
	ATOM	645	CG1	ILE	A	386	16.185	-4.338	0.432	1.00	20.31
	ATOM	646	CD1	ILE	A	386	16.682	-5.766	0.284	1.00	23.97
	ATOM	647	C	ILE	A	386	14.273	-1.645	-1.598	1.00	16.10
	ATOM	648	O	ILE	A	386	14.993	-0.724	-2.004	1.00	17.42
40	ATOM	649	N	LEU	A	387	13.112	-1.944	-2.167	1.00	17.61
	ATOM	650	CA	LEU	A	387	12.620	-1.173	-3.304	1.00	18.20
	ATOM	651	CB	LEU	A	387	11.359	-1.814	-3.882	1.00	17.51
	ATOM	652	CG	LEU	A	387	11.519	-3.064	-4.747	1.00	26.37
	ATOM	653	CD1	LEU	A	387	10.173	-3.406	-5.395	1.00	24.63
45	ATOM	654	CD2	LEU	A	387	12.589	-2.824	-5.808	1.00	21.58
	ATOM	655	C	LEU	A	387	12.283	0.249	-2.838	1.00	17.60
	ATOM	656	O	LEU	A	387	12.571	1.224	-3.530	1.00	17.15
	ATOM	657	N	MET	A	388	11.677	0.357	-1.660	1.00	17.65
	ATOM	658	CA	MET	A	388	11.286	1.656	-1.121	1.00	18.49
50	ATOM	659	CB	MET	A	388	10.302	1.460	0.034	1.00	19.65
	ATOM	660	CG	MET	A	388	8.893	1.105	-0.435	1.00	15.12
	ATOM	661	SD	MET	A	388	7.744	0.769	0.910	1.00	18.73
	ATOM	662	CE	MET	A	388	6.163	0.908	0.048	1.00	18.34
	ATOM	663	C	MET	A	388	12.451	2.553	-0.691	1.00	22.62
55	ATOM	664	O	MET	A	388	12.417	3.767	-0.928	1.00	22.49
	ATOM	665	N	ILE	A	389	13.482	1.988	-0.064	1.00	21.45
	ATOM	666	CA	ILE	A	389	14.604	2.831	0.331	1.00	18.54
	ATOM	667	CB	ILE	A	389	15.590	2.108	1.299	1.00	19.35
	ATOM	668	CG2	ILE	A	389	16.362	0.998	0.578	1.00	15.50
60	ATOM	669	CG1	ILE	A	389	16.556	3.142	1.889	1.00	21.95
	ATOM	670	CD1	ILE	A	389	17.373	2.658	3.080	1.00	15.86

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5	ATOM	671	C	ILE	A	389	15.333	3.322	-0.922	1.00	18.67
	ATOM	672	O	ILE	A	389	15.813	4.453	-0.970	1.00	19.75
	ATOM	673	N	GLY	A	390	15.410	2.477	-1.943	1.00	20.58
	ATOM	674	CA	GLY	A	390	16.049	2.895	-3.183	1.00	19.33
10	ATOM	675	C	GLY	A	390	15.243	4.021	-3.819	1.00	17.48
	ATOM	676	O	GLY	A	390	15.801	4.994	-4.318	1.00	21.87
	ATOM	677	N	LEU	A	391	13.920	3.888	-3.787	1.00	19.17
	ATOM	678	CA	LEU	A	391	13.018	4.887	-4.343	1.00	21.50
15	ATOM	679	CB	LEU	A	391	11.561	4.420	-4.194	1.00	18.25
	ATOM	680	CG	LEU	A	391	10.480	5.497	-4.342	1.00	21.98
	ATOM	681	CD1	LEU	A	391	10.579	6.156	-5.725	1.00	21.39
	ATOM	682	CD2	LEU	A	391	9.115	4.868	-4.148	1.00	17.15
20	ATOM	683	C	LEU	A	391	13.208	6.216	-3.620	1.00	23.27
	ATOM	684	O	LEU	A	391	13.440	7.255	-4.243	1.00	23.60
	ATOM	685	N	VAL	A	392	13.122	6.170	-2.295	1.00	23.04
	ATOM	686	CA	VAL	A	392	13.282	7.357	-1.469	1.00	24.42
25	ATOM	687	CB	VAL	A	392	13.186	6.993	0.042	1.00	27.38
	ATOM	688	CG1	VAL	A	392	13.733	8.129	0.897	1.00	30.37
	ATOM	689	CG2	VAL	A	392	11.739	6.712	0.414	1.00	23.48
	ATOM	690	C	VAL	A	392	14.626	8.014	-1.754	1.00	27.55
30	ATOM	691	O	VAL	A	392	14.728	9.242	-1.832	1.00	27.50
	ATOM	692	N	TRP	A	393	15.652	7.186	-1.924	1.00	23.65
	ATOM	693	CA	TRP	A	393	16.999	7.670	-2.204	1.00	24.76
	ATOM	694	CB	TRP	A	393	17.977	6.491	-2.199	1.00	22.86
35	ATOM	695	CG	TRP	A	393	19.287	6.784	-2.857	1.00	25.90
	ATOM	696	CD2	TRP	A	393	20.341	7.605	-2.339	1.00	28.09
	ATOM	697	CE2	TRP	A	393	21.375	7.612	-3.302	1.00	29.94
	ATOM	698	CE3	TRP	A	393	20.512	8.335	-1.154	1.00	30.20
40	ATOM	699	CD1	TRP	A	393	19.710	6.339	-4.077	1.00	26.55
	ATOM	700	NE1	TRP	A	393	20.963	6.833	-4.351	1.00	30.64
	ATOM	701	CZ2	TRP	A	393	22.566	8.323	-3.120	1.00	32.43
	ATOM	702	CZ3	TRP	A	393	21.698	9.044	-0.971	1.00	34.58
45	ATOM	703	CH2	TRP	A	393	22.709	9.030	-1.950	1.00	36.54
	ATOM	704	C	TRP	A	393	17.082	8.414	-3.547	1.00	25.02
	ATOM	705	O	TRP	A	393	17.767	9.435	-3.650	1.00	20.97
	ATOM	706	N	ARG	A	394	16.399	7.897	-4.568	1.00	23.06
50	ATOM	707	CA	ARG	A	394	16.412	8.531	-5.890	1.00	25.97
	ATOM	708	CB	ARG	A	394	15.776	7.633	-6.965	1.00	24.05
	ATOM	709	CG	ARG	A	394	16.243	6.195	-7.024	1.00	26.05
	ATOM	710	CD	ARG	A	394	15.830	5.551	-8.352	1.00	22.70
55	ATOM	711	NE	ARG	A	394	14.443	5.071	-8.363	1.00	20.71
	ATOM	712	CZ	ARG	A	394	14.053	3.912	-7.841	1.00	21.26
	ATOM	713	NH1	ARG	A	394	14.944	3.108	-7.267	1.00	20.09
	ATOM	714	NH2	ARG	A	394	12.783	3.544	-7.907	1.00	21.26
60	ATOM	715	C	ARG	A	394	15.622	9.833	-5.879	1.00	23.40
	ATOM	716	O	ARG	A	394	15.889	10.729	-6.677	1.00	28.61
	ATOM	717	N	SER	A	395	14.638	9.924	-4.988	1.00	26.65
	ATOM	718	CA	SER	A	395	13.776	11.104	-4.902	1.00	27.46
65	ATOM	719	CB	SER	A	395	12.395	10.696	-4.382	1.00	26.70
	ATOM	720	OG	SER	A	395	11.916	9.530	-5.029	1.00	22.95
	ATOM	721	C	SER	A	395	14.316	12.240	-4.033	1.00	31.45
	ATOM	722	O	SER	A	395	13.726	13.324	-3.977	1.00	28.11
70	ATOM	723	N	MET	A	396	15.437	11.986	-3.368	1.00	33.83
	ATOM	724	CA	MET	A	396	16.061	12.954	-2.475	1.00	38.83
	ATOM	725	CB	MET	A	396	17.466	12.483	-2.112	1.00	39.47
	ATOM	726	CG	MET	A	396	17.585	11.919	-0.715	1.00	41.37
60	ATOM	727	SD	MET	A	396	19.192	12.262	0.004	1.00	42.20

5	ATOM	728	CE	MET	A	396	20.263	11.996	-1.404	1.00	42.84
	ATOM	729	C	MET	A	396	16.143	14.376	-3.018	1.00	40.69
	ATOM	730	O	MET	A	396	15.637	15.316	-2.403	1.00	38.85
	ATOM	731	N	GLU	A	397	16.794	14.526	-4.166	1.00	42.19
	ATOM	732	CA	GLU	A	397	16.971	15.831	-4.790	1.00	44.80
10	ATOM	733	CB	GLU	A	397	18.184	15.785	-5.729	1.00	46.02
	ATOM	734	CG	GLU	A	397	17.883	15.189	-7.096	1.00	54.42
	ATOM	735	CD	GLU	A	397	19.117	14.665	-7.810	1.00	59.40
	ATOM	736	OE1	GLU	A	397	19.219	13.430	-7.990	1.00	60.63
	ATOM	737	OE2	GLU	A	397	19.980	15.485	-8.196	1.00	62.71
15	ATOM	738	C	GLU	A	397	15.735	16.322	-5.554	1.00	42.94
	ATOM	739	O	GLU	A	397	15.830	17.229	-6.376	1.00	44.68
	ATOM	740	N	HIS	A	398	14.579	15.728	-5.280	1.00	40.82
	ATOM	741	CA	HIS	A	398	13.342	16.118	-5.950	1.00	39.21
	ATOM	742	CB	HIS	A	398	12.924	15.043	-6.956	1.00	39.05
20	ATOM	743	CG	HIS	A	398	13.870	14.886	-8.104	1.00	41.57
	ATOM	744	CD2	HIS	A	398	13.904	15.484	-9.318	1.00	39.28
	ATOM	745	ND1	HIS	A	398	14.940	14.017	-8.074	1.00	41.85
	ATOM	746	CE1	HIS	A	398	15.592	14.086	-9.220	1.00	40.88
	ATOM	747	NE2	HIS	A	398	14.985	14.969	-9.993	1.00	42.30
25	ATOM	748	C	HIS	A	398	12.216	16.332	-4.944	1.00	37.04
	ATOM	749	O	HIS	A	398	11.282	15.535	-4.864	1.00	36.51
	ATOM	750	N	PRO	A	399	12.283	17.427	-4.171	1.00	39.19
	ATOM	751	CD	PRO	A	399	13.328	18.467	-4.198	1.00	35.36
	ATOM	752	CA	PRO	A	399	11.243	17.709	-3.173	1.00	37.10
30	ATOM	753	CB	PRO	A	399	11.603	19.101	-2.654	1.00	37.86
	ATOM	754	CG	PRO	A	399	13.050	19.267	-2.963	1.00	35.83
	ATOM	755	C	PRO	A	399	9.828	17.663	-3.744	1.00	37.02
	ATOM	756	O	PRO	A	399	9.554	18.249	-4.789	1.00	38.52
	ATOM	757	N	GLY	A	400	8.938	16.954	-3.057	1.00	33.58
35	ATOM	758	CA	GLY	A	400	7.559	16.865	-3.503	1.00	32.12
	ATOM	759	C	GLY	A	400	7.230	15.706	-4.428	1.00	32.43
	ATOM	760	O	GLY	A	400	6.063	15.344	-4.574	1.00	33.21
	ATOM	761	N	LYS	A	401	8.237	15.112	-5.055	1.00	31.35
	ATOM	762	CA	LYS	A	401	7.972	14.007	-5.966	1.00	30.75
40	ATOM	763	CB	LYS	A	401	8.235	14.430	-7.415	1.00	35.43
	ATOM	764	CG	LYS	A	401	8.130	15.927	-7.675	1.00	35.15
	ATOM	765	CD	LYS	A	401	9.096	16.353	-8.774	1.00	36.88
	ATOM	766	CE	LYS	A	401	8.733	17.721	-9.331	1.00	36.71
	ATOM	767	NZ	LYS	A	401	7.295	18.027	-9.116	1.00	34.22
45	ATOM	768	C	LYS	A	401	8.768	12.746	-5.677	1.00	30.97
	ATOM	769	O	LYS	A	401	9.809	12.776	-5.006	1.00	27.60
	ATOM	770	N	LEU	A	402	8.256	11.635	-6.197	1.00	27.28
	ATOM	771	CA	LEU	A	402	8.889	10.334	-6.050	1.00	29.07
	ATOM	772	CB	LEU	A	402	7.866	9.294	-5.590	1.00	22.55
50	ATOM	773	CG	LEU	A	402	7.265	9.555	-4.207	1.00	24.94
	ATOM	774	CD1	LEU	A	402	6.126	8.583	-3.937	1.00	19.32
	ATOM	775	CD2	LEU	A	402	8.355	9.416	-3.157	1.00	21.54
	ATOM	776	C	LEU	A	402	9.448	9.948	-7.414	1.00	28.78
	ATOM	777	O	LEU	A	402	8.704	9.836	-8.389	1.00	29.98
55	ATOM	778	N	LEU	A	403	10.761	9.770	-7.487	1.00	27.57
	ATOM	779	CA	LEU	A	403	11.393	9.400	-8.744	1.00	27.17
	ATOM	780	CB	LEU	A	403	12.825	9.937	-8.816	1.00	26.95
	ATOM	781	CG	LEU	A	403	13.401	10.027	-10.238	1.00	30.42
	ATOM	782	CD1	LEU	A	403	14.519	11.046	-10.288	1.00	30.76
60	ATOM	783	CD2	LEU	A	403	13.915	8.665	-10.676	1.00	33.11
	ATOM	784	C	LEU	A	403	11.419	7.891	-8.901	1.00	24.78

5	ATOM	785	O	LEU	A	403	12.428	7.257	-8.619	1.00	24.68
	ATOM	786	N	PHE	A	404	10.306	7.319	-9.344	1.00	23.11
	ATOM	787	CA	PHE	A	404	10.239	5.881	-9.546	1.00	26.93
	ATOM	788	CB	PHE	A	404	8.826	5.470	-9.946	1.00	27.04
	ATOM	789	CG	PHE	A	404	7.850	5.513	-8.816	1.00	27.89
	ATOM	790	CD1	PHE	A	404	7.028	6.623	-8.631	1.00	26.20
	ATOM	791	CD2	PHE	A	404	7.750	4.444	-7.925	1.00	23.10
	ATOM	792	CE1	PHE	A	404	6.116	6.668	-7.573	1.00	25.29
	ATOM	793	CE2	PHE	A	404	6.845	4.481	-6.870	1.00	21.01
	ATOM	794	CZ	PHE	A	404	6.026	5.595	-6.693	1.00	22.91
	ATOM	795	C	PHE	A	404	11.232	5.507	-10.637	1.00	26.04
	ATOM	796	O	PHE	A	404	11.882	4.464	-10.578	1.00	27.27
15	ATOM	797	N	ALA	A	405	11.348	6.383	-11.626	1.00	28.80
	ATOM	798	CA	ALA	A	405	12.271	6.195	-12.740	1.00	29.21
	ATOM	799	CB	ALA	A	405	11.650	5.287	-13.806	1.00	26.89
	ATOM	800	C	ALA	A	405	12.549	7.578	-13.317	1.00	30.23
20	ATOM	801	O	ALA	A	405	11.770	8.508	-13.109	1.00	27.38
	ATOM	802	N	PRO	A	406	13.672	7.737	-14.032	1.00	30.05
	ATOM	803	CD	PRO	A	406	14.712	6.745	-14.352	1.00	26.31
	ATOM	804	CA	PRO	A	406	13.977	9.053	-14.604	1.00	32.10
25	ATOM	805	CB	PRO	A	406	15.232	8.800	-15.438	1.00	31.28
	ATOM	806	CG	PRO	A	406	15.865	7.602	-14.776	1.00	31.44
	ATOM	807	C	PRO	A	406	12.820	9.589	-15.436	1.00	32.58
	ATOM	808	O	PRO	A	406	12.605	10.796	-15.507	1.00	32.58
	ATOM	809	N	ASN	A	407	12.063	8.690	-16.053	1.00	32.86
	ATOM	810	CA	ASN	A	407	10.935	9.119	-16.865	1.00	32.78
	ATOM	811	CB	ASN	A	407	10.950	8.418	-18.228	1.00	34.73
	ATOM	812	CG	ASN	A	407	10.884	6.907	-18.121	1.00	35.37
30	ATOM	813	OD1	ASN	A	407	11.189	6.317	-17.077	1.00	30.24
	ATOM	814	ND2	ASN	A	407	10.486	6.268	-19.215	1.00	34.08
	ATOM	815	C	ASN	A	407	9.605	8.901	-16.166	1.00	34.90
	ATOM	816	O	ASN	A	407	8.549	8.897	-16.798	1.00	36.09
35	ATOM	817	N	LEU	A	408	9.660	8.724	-14.851	1.00	33.56
	ATOM	818	CA	LEU	A	408	8.452	8.544	-14.061	1.00	35.59
	ATOM	819	CB	LEU	A	408	8.141	7.062	-13.851	1.00	33.81
	ATOM	820	CG	LEU	A	408	6.696	6.823	-13.397	1.00	36.44
40	ATOM	821	CD1	LEU	A	408	5.746	7.479	-14.390	1.00	34.14
	ATOM	822	CD2	LEU	A	408	6.406	5.334	-13.287	1.00	32.96
	ATOM	823	C	LEU	A	408	8.607	9.245	-12.717	1.00	38.03
	ATOM	824	O	LEU	A	408	8.880	8.614	-11.695	1.00	36.38
45	ATOM	825	N	LEU	A	409	8.441	10.563	-12.741	1.00	37.87
	ATOM	826	CA	LEU	A	409	8.548	11.395	-11.553	1.00	37.95
	ATOM	827	CB	LEU	A	409	9.373	12.636	-11.877	1.00	39.52
	ATOM	828	CG	LEU	A	409	10.023	13.399	-10.728	1.00	42.46
	ATOM	829	CD1	LEU	A	409	11.100	12.547	-10.082	1.00	43.24
	ATOM	830	CD2	LEU	A	409	10.614	14.691	-11.266	1.00	46.05
	ATOM	831	C	LEU	A	409	7.132	11.792	-11.163	1.00	37.13
	ATOM	832	O	LEU	A	409	6.482	12.546	-11.882	1.00	35.70
50	ATOM	833	N	LEU	A	410	6.654	11.284	-10.030	1.00	35.29
	ATOM	834	CA	LEU	A	410	5.297	11.576	-9.583	1.00	33.33
	ATOM	835	CB	LEU	A	410	4.503	10.277	-9.449	1.00	29.37
	ATOM	836	CG	LEU	A	410	4.645	9.238	-10.560	1.00	32.75
55	ATOM	837	CD1	LEU	A	410	4.026	7.925	-10.104	1.00	29.16
	ATOM	838	CD2	LEU	A	410	3.958	9.744	-11.819	1.00	30.70
	ATOM	839	C	LEU	A	410	5.207	12.332	-8.261	1.00	35.14
	ATOM	840	O	LEU	A	410	6.078	12.214	-7.400	1.00	36.94
60	ATOM	841	N	ASP	A	411	4.141	13.108	-8.105	1.00	34.76
	ATOM										

5	ATOM	842	CA	ASP	A	411	3.933	15.843	-6.873	1.00	35.40
	ATOM	843	CB	ASP	A	411	3.733	15.341	-7.144	1.00	40.02
	ATOM	844	CG	ASP	A	411	2.471	15.645	-7.928	1.00	41.32
	ATOM	845	OD1	ASP	A	411	1.570	14.785	-8.001	1.00	45.03
	ATOM	846	OD2	ASP	A	411	2.383	16.764	-8.474	1.00	45.01
10	ATOM	847	C	ASP	A	411	2.727	13.234	-6.179	1.00	36.10
	ATOM	848	O	ASP	A	411	2.033	12.395	-6.762	1.00	34.08
	ATOM	849	N	ARG	A	412	2.480	13.647	-4.940	1.00	35.99
	ATOM	850	CA	ARG	A	412	1.375	13.099	-4.169	1.00	39.37
	ATOM	851	CB	ARG	A	412	1.260	13.824	-2.825	1.00	39.75
15	ATOM	852	CG	ARG	A	412	0.562	15.168	-2.870	1.00	40.49
	ATOM	853	CD	ARG	A	412	0.454	15.736	-1.465	1.00	40.65
	ATOM	854	NE	ARG	A	412	-0.261	14.826	-0.577	1.00	37.48
	ATOM	855	CZ	ARG	A	412	-1.574	14.855	-0.384	1.00	42.84
	ATOM	856	NH1	ARG	A	412	-2.316	15.754	-1.024	1.00	40.82
20	ATOM	857	NH2	ARG	A	412	-2.150	13.986	0.438	1.00	38.32
	ATOM	858	C	ARG	A	412	0.034	13.108	-4.889	1.00	39.80
	ATOM	859	O	ARG	A	412	-0.775	12.201	-4.706	1.00	39.92
	ATOM	860	N	ASN	A	413	-0.198	14.119	-5.717	1.00	41.64
	ATOM	861	CA	ASN	A	413	-1.458	14.215	-6.440	1.00	43.19
25	ATOM	862	CB	ASN	A	413	-1.518	15.533	-7.210	1.00	46.44
	ATOM	863	CG	ASN	A	413	-1.739	16.718	-6.299	1.00	47.86
	ATOM	864	OD1	ASN	A	413	-2.376	16.594	-5.249	1.00	48.05
	ATOM	865	ND2	ASN	A	413	-1.213	17.876	-6.687	1.00	49.43
	ATOM	866	C	ASN	A	413	-1.673	13.044	-7.385	1.00	41.48
30	ATOM	867	O	ASN	A	413	-2.792	12.567	-7.546	1.00	40.50
	ATOM	868	N	GLN	A	414	-0.600	12.577	-8.010	1.00	42.82
	ATOM	869	CA	GLN	A	414	-0.703	11.448	-8.925	1.00	44.73
	ATOM	870	CB	GLN	A	414	0.585	11.307	-9.741	1.00	47.52
	ATOM	871	CG	GLN	A	414	0.572	12.088	-11.049	1.00	50.47
35	ATOM	872	CD	GLN	A	414	1.914	12.713	-11.375	1.00	53.91
	ATOM	873	OE1	GLN	A	414	2.591	13.257	-10.501	1.00	53.68
	ATOM	874	NE2	GLN	A	414	2.309	12.637	-12.641	1.00	56.91
	ATOM	875	C	GLN	A	414	-0.970	10.163	-8.141	1.00	43.21
	ATOM	876	O	GLN	A	414	-1.491	9.193	-8.682	1.00	42.33
40	ATOM	877	N	GLY	A	415	-0.618	10.168	-6.860	1.00	41.97
	ATOM	878	CA	GLY	A	415	-0.836	8.992	-6.040	1.00	40.43
	ATOM	879	C	GLY	A	415	-2.306	8.720	-5.804	1.00	40.80
	ATOM	880	O	GLY	A	415	-2.696	7.601	-5.472	1.00	37.83
	ATOM	881	N	LYS	A	416	-3.129	9.748	-5.978	1.00	42.16
45	ATOM	882	CA	LYS	A	416	-4.566	9.613	-5.779	1.00	44.34
	ATOM	883	CB	LYS	A	416	-5.212	10.996	-5.704	1.00	45.65
	ATOM	884	CG	LYS	A	416	-4.761	11.819	-4.510	1.00	47.42
	ATOM	885	CD	LYS	A	416	-4.910	13.309	-4.777	1.00	50.97
	ATOM	886	CE	LYS	A	416	-5.992	13.924	-3.898	1.00	53.25
50	ATOM	887	NZ	LYS	A	416	-5.416	14.764	-2.809	1.00	56.95
	ATOM	888	C	LYS	A	416	-5.227	8.793	-6.886	1.00	45.33
	ATOM	889	O	LYS	A	416	-6.339	8.299	-6.714	1.00	46.50
	ATOM	890	N	CYS	A	417	-4.540	8.648	-8.015	1.00	45.18
	ATOM	891	CA	CYS	A	417	-5.066	7.890	-9.148	1.00	46.25
55	ATOM	892	CB	CYS	A	417	-4.062	7.902	-10.305	1.00	49.29
	ATOM	893	SG	CYS	A	417	-3.916	9.493	-11.168	1.00	49.59
	ATOM	894	C	CYS	A	417	-5.373	6.452	-8.752	1.00	47.18
	ATOM	895	O	CYS	A	417	-6.220	5.794	-9.359	1.00	46.50
	ATOM	896	N	VAL	A	418	-4.671	5.968	-7.731	1.00	45.07
60	ATOM	897	CA	VAL	A	418	-4.866	4.612	-7.232	1.00	42.75
	ATOM	898	CB	VAL	A	418	-3.525	3.841	-7.206	1.00	42.45

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5	ATOM	899	CG1	VAL	A	418	-3.670	2.563	-6.410	1.00	40.22
	ATOM	900	CG2	VAL	A	418	-3.071	3.538	-8.634	1.00	38.03
	ATOM	901	C	VAL	A	418	-5.441	4.714	-5.818	1.00	41.46
	ATOM	902	O	VAL	A	418	-4.883	5.400	-4.963	1.00	42.08
	ATOM	903	N	GLU	A	419	-6.559	4.036	-5.579	1.00	40.95
10	ATOM	904	CA	GLU	A	419	-7.223	4.073	-4.275	1.00	42.51
	ATOM	905	CB	GLU	A	419	-8.536	3.282	-4.333	1.00	44.52
	ATOM	906	CG	GLU	A	419	-9.010	2.751	-2.984	1.00	50.42
	ATOM	907	CD	GLU	A	419	-10.413	2.168	-3.035	1.00	54.38
	ATOM	908	OE1	GLU	A	419	-10.582	1.059	-3.590	1.00	54.09
15	ATOM	909	OE2	GLU	A	419	-11.347	2.820	-2.516	1.00	57.90
	ATOM	910	C	GLU	A	419	-6.370	3.552	-3.121	1.00	41.11
	ATOM	911	O	GLU	A	419	-5.955	2.393	-3.116	1.00	39.42
	ATOM	912	N	GLY	A	420	-6.129	4.419	-2.140	1.00	40.53
	ATOM	913	CA	GLY	A	420	-5.346	4.049	-0.973	1.00	37.61
20	ATOM	914	C	GLY	A	420	-3.854	4.258	-1.140	1.00	37.01
	ATOM	915	O	GLY	A	420	-3.088	4.105	-0.190	1.00	32.59
	ATOM	916	N	MET	A	421	-3.444	4.623	-2.350	1.00	36.21
	ATOM	917	CA	MET	A	421	-2.035	4.825	-2.656	1.00	36.02
	ATOM	918	CB	MET	A	421	-1.799	4.607	-4.160	1.00	32.84
25	ATOM	919	CG	MET	A	421	-0.351	4.754	-4.617	1.00	35.82
	ATOM	920	SD	MET	A	421	0.806	3.611	-3.812	1.00	35.57
	ATOM	921	CE	MET	A	421	0.881	2.294	-5.005	1.00	32.51
	ATOM	922	C	MET	A	421	-1.474	6.180	-2.226	1.00	34.93
	ATOM	923	O	MET	A	421	-0.275	6.294	-1.985	1.00	35.17
30	ATOM	924	N	VAL	A	422	-2.319	7.205	-2.118	1.00	33.97
	ATOM	925	CA	VAL	A	422	-1.823	8.520	-1.708	1.00	31.29
	ATOM	926	CB	VAL	A	422	-2.927	9.607	-1.766	1.00	33.14
	ATOM	927	CG1	VAL	A	422	-3.823	9.535	-0.533	1.00	30.10
	ATOM	928	CG2	VAL	A	422	-2.279	10.982	-1.854	1.00	30.08
35	ATOM	929	C	VAL	A	422	-1.231	8.498	-0.296	1.00	32.64
	ATOM	930	O	VAL	A	422	-0.274	9.220	0.002	1.00	28.41
	ATOM	931	N	GLU	A	423	-1.803	7.670	0.571	1.00	31.53
	ATOM	932	CA	GLU	A	423	-1.311	7.558	1.935	1.00	35.99
	ATOM	933	CB	GLU	A	423	-2.190	6.594	2.737	1.00	40.37
40	ATOM	934	CG	GLU	A	423	-3.588	7.129	3.043	1.00	49.41
	ATOM	935	CD	GLU	A	423	-4.438	7.336	1.795	1.00	52.38
	ATOM	936	OE1	GLU	A	423	-5.349	8.188	1.835	1.00	56.91
	ATOM	937	OE2	GLU	A	423	-4.200	6.652	0.776	1.00	54.53
	ATOM	938	C	GLU	A	423	0.127	7.043	1.886	1.00	34.83
45	ATOM	939	O	GLU	A	423	1.007	7.552	2.581	1.00	31.85
	ATOM	940	N	ILE	A	424	0.369	6.038	1.050	1.00	30.17
	ATOM	941	CA	ILE	A	424	1.711	5.488	0.929	1.00	28.99
	ATOM	942	CB	ILE	A	424	1.696	4.195	0.109	1.00	30.96
	ATOM	943	CG2	ILE	A	424	3.108	3.588	0.068	1.00	27.20
50	ATOM	944	CG1	ILE	A	424	0.671	3.230	0.725	1.00	30.77
	ATOM	945	CD1	ILE	A	424	0.810	1.787	0.291	1.00	34.69
	ATOM	946	C	ILE	A	424	2.700	6.483	0.312	1.00	28.21
	ATOM	947	O	ILE	A	424	3.856	6.551	0.735	1.00	28.48
	ATOM	948	N	PHE	A	425	2.253	7.260	-0.675	1.00	27.68
55	ATOM	949	CA	PHE	A	425	3.119	8.253	-1.315	1.00	27.30
	ATOM	950	CB	PHE	A	425	2.381	8.958	-2.458	1.00	26.36
	ATOM	951	CG	PHE	A	425	2.538	8.289	-3.798	1.00	27.22
	ATOM	952	CD1	PHE	A	425	2.619	9.050	-4.958	1.00	27.36
	ATOM	953	CD2	PHE	A	425	2.566	6.900	-3.905	1.00	27.89
60	ATOM	954	CE1	PHE	A	425	2.721	8.443	-6.207	1.00	29.63
	ATOM	955	CE2	PHE	A	425	2.668	6.282	-5.149	1.00	27.28



5	ATOM	956	CZ	PHE	A	425	2.745	9.306	-0.312	1.00	27.63
	ATOM	957	C	PHE	A	425	3.591	9.306	-0.312	1.00	25.66
	ATOM	958	O	PHE	A	425	4.757	9.713	-0.328	1.00	26.33
	ATOM	959	N	ASP	A	426	2.680	9.746	0.552	1.00	27.92
	ATOM	960	CA	ASP	A	426	2.984	10.759	1.570	1.00	28.88
10	ATOM	961	CB	ASP	A	426	1.721	11.102	2.369	1.00	32.58
	ATOM	962	CG	ASP	A	426	0.781	12.034	1.613	1.00	37.47
	ATOM	963	OD1	ASP	A	426	-0.432	12.039	1.925	1.00	37.72
	ATOM	964	OD2	ASP	A	426	1.253	12.758	0.710	1.00	36.35
	ATOM	965	C	ASP	A	426	4.071	10.278	2.532	1.00	26.96
15	ATOM	966	O	ASP	A	426	4.974	11.030	2.900	1.00	27.20
	ATOM	967	N	MET	A	427	3.978	9.022	2.947	1.00	25.76
	ATOM	968	CA	MET	A	427	4.981	8.468	3.856	1.00	25.89
	ATOM	969	CB	MET	A	427	4.567	7.070	4.309	1.00	21.17
	ATOM	970	CG	MET	A	427	3.385	7.072	5.257	1.00	24.38
20	ATOM	971	SD	MET	A	427	3.153	5.489	6.080	1.00	34.32
	ATOM	972	CE	MET	A	427	2.173	4.637	4.910	1.00	21.03
	ATOM	973	C	MET	A	427	6.321	8.410	3.128	1.00	22.29
	ATOM	974	O	MET	A	427	7.363	8.760	3.689	1.00	22.19
	ATOM	975	N	LEU	A	428	6.285	7.985	1.868	1.00	21.75
25	ATOM	976	CA	LEU	A	428	7.506	7.892	1.075	1.00	22.91
	ATOM	977	CB	LEU	A	428	7.202	7.252	-0.287	1.00	18.47
	ATOM	978	CG	LEU	A	428	6.910	5.747	-0.176	1.00	19.24
	ATOM	979	CD1	LEU	A	428	6.278	5.222	-1.468	1.00	16.82
	ATOM	980	CD2	LEU	A	428	8.204	5.010	0.131	1.00	16.23
30	ATOM	981	C	LEU	A	428	8.148	9.269	0.902	1.00	23.98
	ATOM	982	O	LEU	A	428	9.366	9.416	1.034	1.00	23.06
	ATOM	983	N	LEU	A	429	7.328	10.281	0.628	1.00	23.91
	ATOM	984	CA	LEU	A	429	7.837	11.642	0.462	1.00	26.29
	ATOM	985	CB	LEU	A	429	6.714	12.571	-0.003	1.00	27.47
35	ATOM	986	CG	LEU	A	429	6.331	12.411	-1.476	1.00	30.78
	ATOM	987	CD1	LEU	A	429	5.022	13.139	-1.751	1.00	34.75
	ATOM	988	CD2	LEU	A	429	7.449	12.952	-2.350	1.00	31.96
	ATOM	989	C	LEU	A	429	8.425	12.166	1.776	1.00	25.83
	ATOM	990	O	LEU	A	429	9.482	12.808	1.793	1.00	26.42
40	ATOM	991	N	ALA	A	430	7.734	11.890	2.877	1.00	26.45
	ATOM	992	CA	ALA	A	430	8.201	12.333	4.185	1.00	26.11
	ATOM	993	CB	ALA	A	430	7.214	11.909	5.265	1.00	23.13
	ATOM	994	C	ALA	A	430	9.577	11.742	4.462	1.00	25.01
	ATOM	995	O	ALA	A	430	10.455	12.409	5.005	1.00	24.31
45	ATOM	996	N	THR	A	431	9.767	10.486	4.074	1.00	25.25
	ATOM	997	CA	THR	A	431	11.046	9.825	4.294	1.00	22.78
	ATOM	998	CB	THR	A	431	10.973	8.323	3.962	1.00	21.36
	ATOM	999	OG1	THR	A	431	9.924	7.727	4.727	1.00	20.27
	ATOM	1000	CG2	THR	A	431	12.291	7.633	4.299	1.00	19.99
50	ATOM	1001	C	THR	A	431	12.103	10.477	3.429	1.00	23.73
	ATOM	1002	O	THR	A	431	13.234	10.667	3.868	1.00	19.60
	ATOM	1003	N	SER	A	432	11.736	10.819	2.197	1.00	24.32
	ATOM	1004	CA	SER	A	432	12.676	11.479	1.301	1.00	26.96
	ATOM	1005	CB	SER	A	432	12.067	11.650	-0.093	1.00	28.70
55	ATOM	1006	OG	SER	A	432	13.084	11.930	-1.039	1.00	33.42
	ATOM	1007	C	SER	A	432	13.033	12.850	1.876	1.00	27.92
	ATOM	1008	O	SER	A	432	14.176	13.294	1.779	1.00	30.78
	ATOM	1009	N	SER	A	433	12.045	13.521	2.459	1.00	28.96
	ATOM	1010	CA	SER	A	433	12.269	14.824	3.076	1.00	34.21
60	ATOM	1011	CB	SER	A	433	10.957	15.387	3.623	1.00	35.07
	ATOM	1012	OG	SER	A	433	10.175	15.961	2.591	1.00	42.38

5	ATOM	1013	C	SER	A	433	13.263	14.644	4.223	1.00	33.43
	ATOM	1014	O	SER	A	433	14.152	15.473	4.429	1.00	31.94
	ATOM	1015	N	ARG	A	434	13.105	13.545	4.959	1.00	31.32
	ATOM	1016	CA	ARG	A	434	13.980	13.236	6.086	1.00	29.78
	ATOM	1017	CB	ARG	A	434	13.468	11.994	6.819	1.00	29.84
10	ATOM	1018	CG	ARG	A	434	14.331	11.541	7.983	1.00	32.17
	ATOM	1019	CD	ARG	A	434	14.626	12.672	8.958	1.00	37.00
	ATOM	1020	NE	ARG	A	434	15.321	12.169	10.140	1.00	39.44
	ATOM	1021	CZ	ARG	A	434	15.935	12.935	11.034	1.00	44.06
	ATOM	1022	NH1	ARG	A	434	15.949	14.255	10.885	1.00	45.52
15	ATOM	1023	NH2	ARG	A	434	16.528	12.381	12.084	1.00	45.01
	ATOM	1024	C	ARG	A	434	15.413	13.014	5.605	1.00	29.24
	ATOM	1025	O	ARG	A	434	16.352	13.563	6.173	1.00	29.72
	ATOM	1026	N	PHE	A	435	15.577	12.206	4.561	1.00	28.95
	ATOM	1027	CA	PHE	A	435	16.901	11.935	4.000	1.00	30.59
20	ATOM	1028	CB	PHE	A	435	16.777	11.045	2.758	1.00	32.03
	ATOM	1029	CG	PHE	A	435	16.795	9.563	3.051	1.00	31.88
	ATOM	1030	CD1	PHE	A	435	16.758	9.084	4.359	1.00	35.60
	ATOM	1031	CD2	PHE	A	435	16.847	8.643	2.009	1.00	35.89
	ATOM	1032	CE1	PHE	A	435	16.771	7.709	4.622	1.00	35.36
25	ATOM	1033	CE2	PHE	A	435	16.860	7.271	2.262	1.00	32.71
	ATOM	1034	CZ	PHE	A	435	16.821	6.807	3.570	1.00	33.24
	ATOM	1035	C	PHE	A	435	17.576	13.253	3.607	1.00	32.73
	ATOM	1036	O	PHE	A	435	18.763	13.464	3.871	1.00	31.16
	ATOM	1037	N	ARG	A	436	16.812	14.137	2.975	1.00	33.37
30	ATOM	1038	CA	ARG	A	436	17.341	15.429	2.549	1.00	39.13
	ATOM	1039	CB	ARG	A	436	16.282	16.206	1.756	1.00	40.42
	ATOM	1040	CG	ARG	A	436	16.846	17.317	0.877	1.00	43.09
	ATOM	1041	CD	ARG	A	436	15.750	17.960	0.040	1.00	44.53
	ATOM	1042	NE	ARG	A	436	14.826	16.955	-0.472	1.00	48.34
35	ATOM	1043	CZ	ARG	A	436	13.530	16.913	-0.184	1.00	48.81
	ATOM	1044	NH1	ARG	A	436	12.997	17.823	0.619	1.00	47.80
	ATOM	1045	NH2	ARG	A	436	12.769	15.950	-0.687	1.00	49.53
	ATOM	1046	C	ARG	A	436	17.792	16.250	3.753	1.00	38.10
	ATOM	1047	O	ARG	A	436	18.896	16.789	3.764	1.00	41.00
40	ATOM	1048	N	MET	A	437	16.936	16.334	4.766	1.00	39.47
	ATOM	1049	CA	MET	A	437	17.257	17.087	5.975	1.00	38.20
	ATOM	1050	CB	MET	A	437	16.102	16.998	6.965	1.00	39.79
	ATOM	1051	C	MET	A	437	18.550	16.594	6.626	1.00	41.15
	ATOM	1052	O	MET	A	437	19.303	17.378	7.201	1.00	40.20
45	ATOM	1053	N	MET	A	438	18.804	15.285	6.538	1.00	39.65
	ATOM	1054	CA	MET	A	438	20.011	14.693	7.117	1.00	39.70
	ATOM	1055	CB	MET	A	438	19.787	13.221	7.463	1.00	39.90
	ATOM	1056	CG	MET	A	438	18.694	12.938	8.460	1.00	41.94
	ATOM	1057	SD	MET	A	438	18.747	11.188	8.880	1.00	43.12
50	ATOM	1058	CE	MET	A	438	20.374	11.064	9.619	1.00	43.73
	ATOM	1059	C	MET	A	438	21.176	14.756	6.142	1.00	38.03
	ATOM	1060	O	MET	A	438	22.321	14.503	6.522	1.00	38.39
	ATOM	1061	N	ASN	A	439	20.886	15.070	4.895	1.00	37.64
	ATOM	1062	CA	ASN	A	439	21.924	15.118	3.895	1.00	35.68
55	ATOM	1063	CB	ASN	A	439	23.019	16.125	4.243	1.00	40.98
	ATOM	1064	CG	ASN	A	439	23.933	16.407	3.090	1.00	45.09
	ATOM	1065	OD1	ASN	A	439	23.528	16.295	1.934	1.00	47.16
	ATOM	1066	ND2	ASN	A	439	25.197	16.733	3.372	1.00	46.87
	ATOM	1067	C	ASN	A	439	22.552	13.732	3.739	1.00	31.06
60	ATOM	1068	O	ASN	A	439	23.764	13.581	3.649	1.00	29.54
	ATOM	1069	N	LEU	A	440	21.692	12.698	3.704	1.00	31.47

5	ATOM	1070	CA	LEU	A	440	22.161	11.326	3.579	1.00	31.63
	ATOM	1071	CB	LEU	A	440	20.991	10.344	3.380	1.00	33.05
	ATOM	1072	CG	LEU	A	440	21.451	8.886	3.209	1.00	37.07
	ATOM	1073	CD1	LEU	A	440	21.957	8.353	4.546	1.00	36.18
	ATOM	1074	CD2	LEU	A	440	20.318	8.032	2.682	1.00	32.33
10	ATOM	1075	C	LEU	A	440	23.146	11.161	2.435	1.00	32.10
	ATOM	1076	O	LEU	A	440	22.925	11.671	1.333	1.00	32.76
	ATOM	1077	N	GLN	A	441	24.225	10.450	2.702	1.00	32.54
	ATOM	1078	CA	GLN	A	441	25.255	10.220	1.699	1.00	31.97
	ATOM	1079	CB	GLN	A	441	26.632	10.320	2.345	1.00	31.75
15	ATOM	1080	CG	GLN	A	441	26.896	11.669	2.979	1.00	35.56
	ATOM	1081	CD	GLN	A	441	27.040	12.748	1.939	1.00	34.97
	ATOM	1082	OE1	GLN	A	441	27.985	12.782	1.167	1.00	35.51
	ATOM	1083	NE2	GLN	A	441	26.053	13.659	1.899	1.00	35.41
	ATOM	1084	C	GLN	A	441	25.100	8.860	1.038	1.00	34.08
20	ATOM	1085	O	GLN	A	441	24.540	7.931	1.625	1.00	30.73
	ATOM	1086	N	GLY	A	442	25.608	8.752	-0.187	1.00	32.78
	ATOM	1087	CA	GLY	A	442	25.528	7.503	-0.921	1.00	32.91
	ATOM	1088	C	GLY	A	442	26.181	6.350	-0.184	1.00	31.87
	ATOM	1089	O	GLY	A	442	25.642	5.245	-0.154	1.00	33.18
25	ATOM	1090	N	GLU	A	443	27.340	6.603	0.416	1.00	30.60
	ATOM	1091	CA	GLU	A	443	28.057	5.567	1.150	1.00	30.85
	ATOM	1092	CB	GLU	A	443	29.376	6.111	1.704	1.00	32.74
	ATOM	1093	CG	GLU	A	443	30.425	6.378	0.646	1.00	36.30
	ATOM	1094	CD	GLU	A	443	30.310	7.770	0.066	1.00	40.92
30	ATOM	1095	OE1	GLU	A	443	29.677	8.630	0.716	1.00	42.27
	ATOM	1096	OE2	GLU	A	443	30.853	8.003	-1.038	1.00	46.82
	ATOM	1097	C	GLU	A	443	27.206	5.048	2.299	1.00	30.43
	ATOM	1098	O	GLU	A	443	27.211	3.854	2.595	1.00	28.11
	ATOM	1099	N	GLU	A	444	26.482	5.955	2.948	1.00	30.26
35	ATOM	1100	CA	GLU	A	444	25.619	5.589	4.067	1.00	28.18
	ATOM	1101	CB	GLU	A	444	25.147	6.843	4.797	1.00	26.32
	ATOM	1102	CG	GLU	A	444	26.250	7.633	5.463	1.00	29.27
	ATOM	1103	CD	GLU	A	444	25.748	8.944	6.023	1.00	29.62
	ATOM	1104	OE1	GLU	A	444	25.006	9.652	5.304	1.00	32.00
40	ATOM	1105	OE2	GLU	A	444	26.088	9.268	7.182	1.00	29.02
	ATOM	1106	C	GLU	A	444	24.403	4.813	3.572	1.00	26.93
	ATOM	1107	O	GLU	A	444	23.970	3.841	4.191	1.00	24.78
	ATOM	1108	N	PHE	A	445	23.861	5.256	2.443	1.00	27.79
	ATOM	1109	CA	PHE	A	445	22.688	4.633	1.853	1.00	24.50
45	ATOM	1110	CB	PHE	A	445	22.254	5.416	0.610	1.00	25.40
	ATOM	1111	CG	PHE	A	445	21.372	4.634	-0.316	1.00	23.74
	ATOM	1112	CD1	PHE	A	445	20.034	4.419	-0.004	1.00	23.00
	ATOM	1113	CD2	PHE	A	445	21.885	4.094	-1.489	1.00	22.37
	ATOM	1114	CE1	PHE	A	445	19.215	3.670	-0.855	1.00	22.57
50	ATOM	1115	CE2	PHE	A	445	21.079	3.349	-2.342	1.00	21.69
	ATOM	1116	CZ	PHE	A	445	19.741	3.138	-2.023	1.00	22.25
	ATOM	1117	C	PHE	A	445	22.913	3.169	1.489	1.00	22.81
	ATOM	1118	O	PHE	A	445	22.083	2.316	1.796	1.00	22.92
	ATOM	1119	N	VAL	A	446	24.019	2.868	0.822	1.00	22.46
55	ATOM	1120	CA	VAL	A	446	24.278	1.481	0.447	1.00	22.26
	ATOM	1121	CB	VAL	A	446	25.522	1.360	-0.465	1.00	22.87
	ATOM	1122	CG1	VAL	A	446	25.251	2.046	-1.799	1.00	22.57
	ATOM	1123	CG2	VAL	A	446	26.735	1.968	0.217	1.00	22.38
	ATOM	1124	C	VAL	A	446	24.467	0.614	1.694	1.00	23.68
60	ATOM	1125	O	VAL	A	446	24.177	-0.586	1.680	1.00	22.91
	ATOM	1126	N	CYS	A	447	24.962	1.223	2.770	1.00	22.02

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5	ATOM	1184	CD2	LEU	A	454	22.785	-9.913	4.952	1.00	22.84
	ATOM	1185	C	LEU	A	454	19.572	-8.945	7.807	1.00	26.06
	ATOM	1186	O	LEU	A	454	19.413	-9.997	8.438	1.00	27.44
	ATOM	1187	N	ASN	A	455	19.011	-7.795	8.167	1.00	25.01
	ATOM	1188	CA	ASN	A	455	18.240	-7.681	9.400	1.00	26.10
10	ATOM	1189	CB	ASN	A	455	18.439	-6.295	10.002	1.00	22.67
	ATOM	1190	CG	ASN	A	455	17.627	-6.109	11.264	1.00	26.67
	ATOM	1191	OD1	ASN	A	455	17.899	-6.751	12.270	1.00	25.16
	ATOM	1192	ND2	ASN	A	455	16.615	-5.246	11.212	1.00	20.73
	ATOM	1193	C	ASN	A	455	16.739	-7.957	9.418	1.00	25.78
15	ATOM	1194	O	ASN	A	455	16.230	-8.516	10.380	1.00	29.22
	ATOM	1195	N	SER	A	456	16.027	-7.549	8.381	1.00	28.51
	ATOM	1196	CA	SER	A	456	14.578	-7.704	8.371	1.00	32.52
	ATOM	1197	CB	SER	A	456	14.019	-7.213	7.033	1.00	35.98
	ATOM	1198	OG	SER	A	456	14.266	-5.818	6.897	1.00	30.88
20	ATOM	1199	C	SER	A	456	14.033	-9.086	8.711	1.00	33.00
	ATOM	1200	O	SER	A	456	13.112	-9.202	9.523	1.00	33.07
	ATOM	1201	N	GLY	A	457	14.597	-10.130	8.117	1.00	28.40
	ATOM	1202	CA	GLY	A	457	14.115	-11.464	8.413	1.00	36.28
	ATOM	1203	C	GLY	A	457	15.055	-12.289	9.277	1.00	40.41
25	ATOM	1204	O	GLY	A	457	14.831	-13.486	9.456	1.00	38.20
	ATOM	1205	N	VAL	A	458	16.095	-11.657	9.820	1.00	44.13
	ATOM	1206	CA	VAL	A	458	17.079	-12.356	10.647	1.00	51.09
	ATOM	1207	CB	VAL	A	458	18.214	-11.399	11.095	1.00	51.06
	ATOM	1208	CG1	VAL	A	458	17.688	-10.390	12.104	1.00	51.75
30	ATOM	1209	CG2	VAL	A	458	19.365	-12.199	11.692	1.00	50.65
	ATOM	1210	C	VAL	A	458	16.513	-13.060	11.885	1.00	57.26
	ATOM	1211	O	VAL	A	458	17.085	-14.045	12.356	1.00	58.77
	ATOM	1212	N	TYR	A	459	15.401	-12.560	12.416	1.00	62.31
	ATOM	1213	CA	TYR	A	459	14.793	-13.177	13.592	1.00	68.49
35	ATOM	1214	CB	TYR	A	459	14.293	-12.100	14.560	1.00	70.46
	ATOM	1215	CG	TYR	A	459	15.396	-11.196	15.069	1.00	71.73
	ATOM	1216	CD1	TYR	A	459	15.127	-9.888	15.462	1.00	71.93
	ATOM	1217	CE1	TYR	A	459	16.147	-9.045	15.898	1.00	72.60
	ATOM	1218	CD2	TYR	A	459	16.716	-11.644	15.128	1.00	72.77
40	ATOM	1219	CE2	TYR	A	459	17.741	-10.812	15.560	1.00	73.55
	ATOM	1220	CZ	TYR	A	459	17.450	-9.514	15.941	1.00	72.93
	ATOM	1221	OH	TYR	A	459	18.467	-8.687	16.351	1.00	74.56
	ATOM	1222	C	TYR	A	459	13.649	-14.097	13.187	1.00	71.86
	ATOM	1223	O	TYR	A	459	13.380	-15.099	13.852	1.00	73.11
45	ATOM	1224	N	THR	A	460	12.981	-13.756	12.090	1.00	74.84
	ATOM	1225	CA	THR	A	460	11.881	-14.567	11.589	1.00	77.66
	ATOM	1226	CB	THR	A	460	11.246	-13.900	10.373	1.00	76.69
	ATOM	1227	C	THR	A	460	12.436	-15.938	11.212	1.00	80.26
	ATOM	1228	O	THR	A	460	11.684	-16.866	10.912	1.00	80.82
50	ATOM	1229	N	PHE	A	461	13.762	-16.051	11.231	1.00	82.69
	ATOM	1230	CA	PHE	A	461	14.440	-17.299	10.905	1.00	85.63
	ATOM	1231	CB	PHE	A	461	15.920	-17.034	10.630	1.00	85.47
	ATOM	1232	C	PHE	A	461	14.284	-18.288	12.059	1.00	87.52
	ATOM	1233	O	PHE	A	461	14.493	-17.940	13.224	1.00	86.53
55	ATOM	1234	N	LEU	A	462	13.914	-19.520	11.724	1.00	89.49
	ATOM	1235	CA	LEU	A	462	13.711	-20.568	12.718	1.00	91.34
	ATOM	1236	CB	LEU	A	462	12.961	-21.741	12.087	1.00	91.23
	ATOM	1237	C	LEU	A	462	15.016	-21.060	13.340	1.00	92.05
	ATOM	1238	O	LEU	A	462	16.042	-21.165	12.664	1.00	91.91
60	ATOM	1239	N	SER	A	463	14.966	-21.357	14.635	1.00	92.53
	ATOM	1240	CA	SER	A	463	16.131	-21.855	15.358	1.00	92.96

5	ATOM	1241	CB	SER	A	463	16.033	-21.483	16.833	1.00	91.67
	ATOM	1242	C	SER	A	463	16.189	-23.371	15.200	1.00	93.39
	ATOM	1243	O	SER	A	463	15.156	-24.034	15.102	1.00	93.44
	ATOM	1244	N	SER	A	464	17.399	-23.917	15.167	1.00	93.82
	ATOM	1245	CA	SER	A	464	17.577	-25.355	15.015	1.00	93.85
10	ATOM	1246	CB	SER	A	464	17.284	-25.769	13.577	1.00	93.74
	ATOM	1247	C	SER	A	464	18.997	-25.743	15.396	1.00	93.96
	ATOM	1248	O	SER	A	464	19.815	-26.074	14.535	1.00	93.65
	ATOM	1249	N	THR	A	465	19.279	-25.699	16.694	1.00	93.91
	ATOM	1250	CA	THR	A	465	20.600	-26.036	17.212	1.00	93.79
15	ATOM	1251	CB	THR	A	465	20.952	-27.483	16.863	1.00	93.38
	ATOM	1252	C	THR	A	465	21.640	-25.085	16.634	1.00	93.27
	ATOM	1253	O	THR	A	465	21.302	-24.017	16.121	1.00	93.03
	ATOM	1254	N	LEU	A	466	22.907	-25.479	16.723	1.00	93.26
	ATOM	1255	CA	LEU	A	466	23.999	-24.665	16.207	1.00	92.34
20	ATOM	1256	CB	LEU	A	466	25.335	-25.338	16.498	1.00	91.59
	ATOM	1257	C	LEU	A	466	23.829	-24.461	14.706	1.00	92.18
	ATOM	1258	O	LEU	A	466	24.411	-23.545	14.125	1.00	92.67
	ATOM	1259	N	LYS	A	467	23.028	-25.323	14.086	1.00	91.28
	ATOM	1260	CA	LYS	A	467	22.772	-25.238	12.653	1.00	90.02
25	ATOM	1261	CB	LYS	A	467	21.740	-26.287	12.240	1.00	89.93
	ATOM	1262	C	LYS	A	467	22.269	-23.841	12.308	1.00	88.35
	ATOM	1263	O	LYS	A	467	23.032	-22.990	11.849	1.00	88.50
	ATOM	1264	N	SER	A	468	20.981	-23.610	12.536	1.00	86.02
	ATOM	1265	CA	SER	A	468	20.384	-22.315	12.252	1.00	84.10
30	ATOM	1266	CB	SER	A	468	18.901	-22.333	12.620	1.00	84.08
	ATOM	1267	OG	SER	A	468	18.229	-23.378	11.937	1.00	83.03
	ATOM	1268	C	SER	A	468	21.109	-21.230	13.040	1.00	83.39
	ATOM	1269	O	SER	A	468	21.264	-20.105	12.565	1.00	83.48
	ATOM	1270	N	LEU	A	469	21.558	-21.579	14.242	1.00	82.04
35	ATOM	1271	CA	LEU	A	469	22.276	-20.640	15.098	1.00	80.28
	ATOM	1272	CB	LEU	A	469	22.595	-21.294	16.436	1.00	79.81
	ATOM	1273	C	LEU	A	469	23.564	-20.174	14.419	1.00	79.18
	ATOM	1274	O	LEU	A	469	24.111	-19.122	14.756	1.00	78.61
	ATOM	1275	N	GLU	A	470	24.044	-20.969	13.466	1.00	76.69
40	ATOM	1276	CA	GLU	A	470	25.256	-20.638	12.726	1.00	74.84
	ATOM	1277	CB	GLU	A	470	25.803	-21.880	12.032	1.00	74.12
	ATOM	1278	C	GLU	A	470	24.920	-19.565	11.697	1.00	73.77
	ATOM	1279	O	GLU	A	470	25.617	-18.556	11.581	1.00	72.94
	ATOM	1280	N	GLU	A	471	23.842	-19.792	10.953	1.00	72.08
45	ATOM	1281	CA	GLU	A	471	23.396	-18.842	9.945	1.00	70.05
	ATOM	1282	CB	GLU	A	471	22.461	-19.526	8.944	1.00	71.52
	ATOM	1283	CG	GLU	A	471	23.150	-19.976	7.668	1.00	72.90
	ATOM	1284	CD	GLU	A	471	24.512	-20.586	7.932	1.00	74.01
	ATOM	1285	OE1	GLU	A	471	25.469	-20.258	7.198	1.00	74.22
50	ATOM	1286	OE2	GLU	A	471	24.626	-21.395	8.878	1.00	75.18
	ATOM	1287	C	GLU	A	471	22.667	-17.692	10.630	1.00	67.33
	ATOM	1288	O	GLU	A	471	21.685	-17.165	10.107	1.00	67.77
	ATOM	1289	N	LYS	A	472	23.152	-17.319	11.811	1.00	62.63
	ATOM	1290	CA	LYS	A	472	22.564	-16.229	12.578	1.00	57.41
55	ATOM	1291	CB	LYS	A	472	21.697	-16.777	13.713	1.00	58.74
	ATOM	1292	CG	LYS	A	472	20.683	-15.776	14.243	1.00	60.32
	ATOM	1293	CD	LYS	A	472	19.271	-16.342	14.219	1.00	60.73
	ATOM	1294	CE	LYS	A	472	18.485	-15.909	15.449	1.00	61.78
	ATOM	1295	NZ	LYS	A	472	19.352	-15.788	16.658	1.00	60.09
60	ATOM	1296	C	LYS	A	472	23.662	-15.339	13.150	1.00	53.42
	ATOM	1297	O	LYS	A	472	23.631	-14.120	12.978	1.00	50.87

5	ATOM	1298	N	ASP	A	473	24.628	-15.949	13.830	1.00	47.52
	ATOM	1299	CA	ASP	A	473	25.732	-15.194	14.405	1.00	45.55
	ATOM	1300	CB	ASP	A	473	26.613	-16.094	15.269	1.00	50.48
	ATOM	1301	CG	ASP	A	473	26.380	-15.885	16.749	1.00	55.50
	ATOM	1302	OD1	ASP	A	473	25.272	-15.436	17.118	1.00	58.06
10	ATOM	1303	OD2	ASP	A	473	27.304	-16.170	17.541	1.00	59.81
	ATOM	1304	C	ASP	A	473	26.557	-14.611	13.269	1.00	42.62
	ATOM	1305	O	ASP	A	473	27.087	-13.506	13.373	1.00	42.10
	ATOM	1306	N	HIS	A	474	26.663	-15.364	12.180	1.00	38.05
	ATOM	1307	CA	HIS	A	474	27.416	-14.904	11.026	1.00	37.25
15	ATOM	1308	CB	HIS	A	474	27.429	-15.978	9.941	1.00	35.07
	ATOM	1309	CG	HIS	A	474	28.036	-15.523	8.653	1.00	37.36
	ATOM	1310	CD2	HIS	A	474	29.292	-15.113	8.355	1.00	38.86
	ATOM	1311	ND1	HIS	A	474	27.322	-15.452	7.476	1.00	41.31
	ATOM	1312	CE1	HIS	A	474	28.110	-15.020	6.509	1.00	40.86
20	ATOM	1313	NE2	HIS	A	474	29.311	-14.807	7.016	1.00	44.49
	ATOM	1314	C	HIS	A	474	26.749	-13.640	10.493	1.00	36.68
	ATOM	1315	O	HIS	A	474	27.417	-12.676	10.132	1.00	36.48
	ATOM	1316	N	ILE	A	475	25.422	-13.652	10.447	1.00	35.93
	ATOM	1317	CA	ILE	A	475	24.683	-12.499	9.963	1.00	36.21
25	ATOM	1318	CB	ILE	A	475	23.174	-12.797	9.868	1.00	36.31
	ATOM	1319	CG2	ILE	A	475	22.411	-11.527	9.513	1.00	38.19
	ATOM	1320	CG1	ILE	A	475	22.922	-13.874	8.813	1.00	36.97
	ATOM	1321	CD1	ILE	A	475	21.528	-14.454	8.869	1.00	35.59
	ATOM	1322	C	ILE	A	475	24.893	-11.322	10.907	1.00	35.34
30	ATOM	1323	O	ILE	A	475	25.092	-10.189	10.471	1.00	33.20
	ATOM	1324	N	HIS	A	476	24.857	-11.596	12.206	1.00	35.95
	ATOM	1325	CA	HIS	A	476	25.031	-10.540	13.193	1.00	35.06
	ATOM	1326	CB	HIS	A	476	24.681	-11.062	14.585	1.00	37.30
	ATOM	1327	CG	HIS	A	476	23.210	-11.068	14.860	1.00	43.06
35	ATOM	1328	CD2	HIS	A	476	22.329	-10.051	15.017	1.00	43.93
	ATOM	1329	ND1	HIS	A	476	22.476	-12.230	14.968	1.00	45.60
	ATOM	1330	CE1	HIS	A	476	21.207	-11.928	15.177	1.00	47.56
	ATOM	1331	NE2	HIS	A	476	21.091	-10.613	15.211	1.00	46.21
	ATOM	1332	C	HIS	A	476	26.438	-9.966	13.170	1.00	35.40
40	ATOM	1333	O	HIS	A	476	26.634	-8.774	13.415	1.00	35.45
	ATOM	1334	N	ARG	A	477	27.420	-10.805	12.862	1.00	34.07
	ATOM	1335	CA	ARG	A	477	28.796	-10.331	12.795	1.00	34.18
	ATOM	1336	CB	ARG	A	477	29.757	-11.506	12.605	1.00	41.04
	ATOM	1337	CG	ARG	A	477	29.800	-12.459	13.788	1.00	47.61
45	ATOM	1338	CD	ARG	A	477	30.782	-13.599	13.557	1.00	55.67
	ATOM	1339	NE	ARG	A	477	31.780	-13.675	14.622	1.00	60.17
	ATOM	1340	CZ	ARG	A	477	32.780	-12.811	14.770	1.00	61.98
	ATOM	1341	NH1	ARG	A	477	32.918	-11.803	13.918	1.00	64.29
	ATOM	1342	NH2	ARG	A	477	33.643	-12.955	15.766	1.00	62.79
50	ATOM	1343	C	ARG	A	477	28.906	-9.361	11.621	1.00	30.77
	ATOM	1344	O	ARG	A	477	29.462	-8.268	11.753	1.00	33.59
	ATOM	1345	N	VAL	A	478	28.369	-9.766	10.475	1.00	27.65
	ATOM	1346	CA	VAL	A	478	28.389	-8.930	9.280	1.00	27.07
	ATOM	1347	CB	VAL	A	478	27.658	-9.605	8.100	1.00	28.00
55	ATOM	1348	CG1	VAL	A	478	27.672	-8.678	6.890	1.00	25.83
	ATOM	1349	CG2	VAL	A	478	28.319	-10.933	7.761	1.00	31.66
	ATOM	1350	C	VAL	A	478	27.689	-7.610	9.584	1.00	26.92
	ATOM	1351	O	VAL	A	478	28.216	-6.536	9.294	1.00	26.97
	ATOM	1352	N	LEU	A	479	26.499	-7.702	10.171	1.00	25.74
60	ATOM	1353	CA	LEU	A	479	25.727	-6.516	10.530	1.00	27.97
	ATOM	1354	CB	LEU	A	479	24.474	-6.912	11.324	1.00	25.55

5	ATOM	1355	CG	LEU	A	479	23.211	<del>10.517</del>	10.517	1.00	29.01
	ATOM	1356	CD1	LEU	A	479	22.056	-7.503	11.481	1.00	27.05
	ATOM	1357	CD2	LEU	A	479	22.864	-6.063	9.584	1.00	24.92
	ATOM	1358	C	LEU	A	479	26.592	-5.582	11.369	1.00	25.39
	ATOM	1359	O	LEU	A	479	26.595	-4.370	11.158	1.00	27.39
10	ATOM	1360	N	ASP	A	480	27.324	-6.158	12.320	1.00	26.04
	ATOM	1361	CA	ASP	A	480	28.206	-5.388	13.193	1.00	27.32
	ATOM	1362	CB	ASP	A	480	28.878	-6.305	14.222	1.00	26.67
	ATOM	1363	CG	ASP	A	480	27.990	-6.602	15.417	1.00	31.02
	ATOM	1364	OD1	ASP	A	480	28.355	-7.505	16.198	1.00	31.50
15	ATOM	1365	OD2	ASP	A	480	26.935	-5.944	15.580	1.00	32.21
	ATOM	1366	C	ASP	A	480	29.283	-4.699	12.361	1.00	25.59
	ATOM	1367	O	ASP	A	480	29.672	-3.562	12.636	1.00	27.15
	ATOM	1368	N	LYS	A	481	29.767	-5.394	11.340	1.00	25.17
	ATOM	1369	CA	LYS	A	481	30.794	-4.830	10.477	1.00	24.93
20	ATOM	1370	CB	LYS	A	481	31.306	-5.890	9.512	1.00	28.42
	ATOM	1371	CG	LYS	A	481	32.158	-6.953	10.188	1.00	35.59
	ATOM	1372	CD	LYS	A	481	32.894	-7.799	9.157	1.00	41.21
	ATOM	1373	CE	LYS	A	481	33.883	-6.963	8.350	1.00	41.48
	ATOM	1374	NZ	LYS	A	481	34.954	-6.388	9.215	1.00	43.22
25	ATOM	1375	C	LYS	A	481	30.260	-3.635	9.696	1.00	26.12
	ATOM	1376	O	LYS	A	481	30.979	-2.657	9.463	1.00	23.73
	ATOM	1377	N	ILE	A	482	28.996	-3.705	9.291	1.00	25.44
	ATOM	1378	CA	ILE	A	482	28.421	-2.598	8.545	1.00	27.69
	ATOM	1379	CB	ILE	A	482	27.066	-2.983	7.915	1.00	27.59
30	ATOM	1380	CG2	ILE	A	482	26.470	-1.788	7.183	1.00	25.97
	ATOM	1381	CG1	ILE	A	482	27.274	-4.131	6.922	1.00	23.80
	ATOM	1382	CD1	ILE	A	482	26.000	-4.838	6.533	1.00	21.30
	ATOM	1383	C	ILE	A	482	28.253	-1.408	9.481	1.00	27.33
	ATOM	1384	O	ILE	A	482	28.312	-0.256	9.045	1.00	28.55
35	ATOM	1385	N	THR	A	483	28.046	-1.690	10.768	1.00	25.03
	ATOM	1386	CA	THR	A	483	27.905	-0.632	11.760	1.00	23.62
	ATOM	1387	CB	THR	A	483	27.535	-1.192	13.154	1.00	22.18
	ATOM	1388	OG1	THR	A	483	26.181	-1.658	13.133	1.00	25.39
	ATOM	1389	CG2	THR	A	483	27.673	-0.111	14.226	1.00	25.84
40	ATOM	1390	C	THR	A	483	29.257	0.074	11.858	1.00	23.04
	ATOM	1391	O	THR	A	483	29.331	1.306	11.846	1.00	23.55
	ATOM	1392	N	ASP	A	484	30.324	-0.714	11.960	1.00	22.24
	ATOM	1393	CA	ASP	A	484	31.674	-0.152	12.039	1.00	25.48
	ATOM	1394	CB	ASP	A	484	32.718	-1.273	12.107	1.00	26.88
45	ATOM	1395	CG	ASP	A	484	32.629	-2.083	13.394	1.00	32.52
	ATOM	1396	OD1	ASP	A	484	32.002	-1.608	14.366	1.00	33.68
	ATOM	1397	OD2	ASP	A	484	33.185	-3.198	13.434	1.00	34.63
	ATOM	1398	C	ASP	A	484	31.930	0.715	10.807	1.00	25.16
	ATOM	1399	O	ASP	A	484	32.481	1.812	10.905	1.00	26.05
50	ATOM	1400	N	THR	A	485	31.505	0.226	9.645	1.00	28.96
	ATOM	1401	CA	THR	A	485	31.689	0.960	8.394	1.00	26.63
	ATOM	1402	CB	THR	A	485	31.124	0.166	7.197	1.00	26.12
	ATOM	1403	OG1	THR	A	485	31.753	-1.123	7.132	1.00	24.30
	ATOM	1404	CG2	THR	A	485	31.381	0.907	5.898	1.00	23.31
55	ATOM	1405	C	THR	A	485	30.994	2.318	8.468	1.00	28.90
	ATOM	1406	O	THR	A	485	31.583	3.354	8.137	1.00	27.26
	ATOM	1407	N	LEU	A	486	29.743	2.310	8.915	1.00	24.76
	ATOM	1408	CA	LEU	A	486	28.973	3.537	9.027	1.00	26.19
	ATOM	1409	CB	LEU	A	486	27.567	3.233	9.547	1.00	27.27
60	ATOM	1410	CG	LEU	A	486	26.508	2.921	8.486	1.00	23.50
	ATOM	1411	CD1	LEU	A	486	25.210	2.550	9.183	1.00	22.03



5	ATOM	1412	CD2	LEU	A	486	26.309	4.128	7.577	1.00	21.35
	ATOM	1413	C	LEU	A	486	29.662	4.519	9.960	1.00	27.36
	ATOM	1414	O	LEU	A	486	29.745	5.710	9.669	1.00	25.87
	ATOM	1415	N	ILE	A	487	30.151	4.015	11.088	1.00	27.88
	ATOM	1416	CA	ILE	A	487	30.843	4.857	12.055	1.00	28.40
10	ATOM	1417	CB	ILE	A	487	31.203	4.054	13.332	1.00	26.74
	ATOM	1418	CG2	ILE	A	487	32.255	4.803	14.154	1.00	27.54
	ATOM	1419	CG1	ILE	A	487	29.937	3.813	14.163	1.00	25.93
	ATOM	1420	CD1	ILE	A	487	29.237	5.088	14.624	1.00	23.42
	ATOM	1421	C	ILE	A	487	32.125	5.393	11.412	1.00	28.89
15	ATOM	1422	O	ILE	A	487	32.497	6.554	11.602	1.00	29.85
	ATOM	1423	N	HIS	A	488	32.791	4.533	10.649	1.00	29.71
	ATOM	1424	CA	HIS	A	488	34.031	4.898	9.967	1.00	34.12
	ATOM	1425	CB	HIS	A	488	34.585	3.691	9.207	1.00	36.61
	ATOM	1426	CG	HIS	A	488	35.799	3.997	8.385	1.00	42.74
20	ATOM	1427	CD2	HIS	A	488	35.970	4.089	7.045	1.00	43.12
	ATOM	1428	ND1	HIS	A	488	37.034	4.239	8.946	1.00	43.13
	ATOM	1429	CE1	HIS	A	488	37.913	4.466	7.987	1.00	43.40
	ATOM	1430	NE2	HIS	A	488	37.293	4.381	6.825	1.00	45.63
	ATOM	1431	C	HIS	A	488	33.799	6.051	8.998	1.00	32.74
25	ATOM	1432	O	HIS	A	488	34.577	7.004	8.955	1.00	31.06
	ATOM	1433	N	LEU	A	489	32.721	5.958	8.223	1.00	33.56
	ATOM	1434	CA	LEU	A	489	32.384	6.992	7.258	1.00	30.78
	ATOM	1435	CB	LEU	A	489	31.145	6.587	6.464	1.00	34.67
	ATOM	1436	CG	LEU	A	489	31.310	5.353	5.574	1.00	34.73
30	ATOM	1437	CD1	LEU	A	489	29.945	4.856	5.125	1.00	33.21
	ATOM	1438	CD2	LEU	A	489	32.183	5.701	4.378	1.00	35.92
	ATOM	1439	C	LEU	A	489	32.124	8.320	7.954	1.00	33.97
	ATOM	1440	O	LEU	A	489	32.587	9.365	7.507	1.00	33.22
	ATOM	1441	N	MET	A	490	31.387	8.274	9.058	1.00	31.33
35	ATOM	1442	CA	MET	A	490	31.056	9.482	9.801	1.00	30.61
	ATOM	1443	CB	MET	A	490	30.000	9.161	10.862	1.00	32.34
	ATOM	1444	CG	MET	A	490	28.607	8.940	10.289	1.00	30.71
	ATOM	1445	SD	MET	A	490	27.457	8.247	11.496	1.00	31.14
	ATOM	1446	CE	MET	A	490	26.321	7.408	10.418	1.00	30.36
40	ATOM	1447	C	MET	A	490	32.287	10.108	10.455	1.00	32.22
	ATOM	1448	O	MET	A	490	32.412	11.330	10.517	1.00	28.25
	ATOM	1449	N	ALA	A	491	33.184	9.262	10.949	1.00	33.81
	ATOM	1450	CA	ALA	A	491	34.407	9.730	11.585	1.00	39.92
	ATOM	1451	CB	ALA	A	491	35.168	8.554	12.185	1.00	37.22
45	ATOM	1452	C	ALA	A	491	35.275	10.445	10.550	1.00	42.68
	ATOM	1453	O	ALA	A	491	35.865	11.487	10.838	1.00	45.32
	ATOM	1454	N	LYS	A	492	35.339	9.876	9.347	1.00	44.39
	ATOM	1455	CA	LYS	A	492	36.122	10.440	8.248	1.00	44.80
	ATOM	1456	CB	LYS	A	492	36.136	9.477	7.052	1.00	46.96
50	ATOM	1457	CG	LYS	A	492	37.490	8.840	6.744	1.00	47.20
	ATOM	1458	CD	LYS	A	492	37.390	7.830	5.595	1.00	45.71
	ATOM	1459	CE	LYS	A	492	38.631	6.937	5.518	1.00	45.55
	ATOM	1460	NZ	LYS	A	492	38.357	5.577	4.948	1.00	36.28
	ATOM	1461	C	LYS	A	492	35.534	11.780	7.809	1.00	45.61
55	ATOM	1462	O	LYS	A	492	36.227	12.604	7.215	1.00	46.18
	ATOM	1463	N	ALA	A	493	34.254	11.992	8.100	1.00	43.75
	ATOM	1464	CA	ALA	A	493	33.590	13.238	7.728	1.00	42.42
	ATOM	1465	CB	ALA	A	493	32.097	13.001	7.528	1.00	40.92
	ATOM	1466	C	ALA	A	493	33.816	14.305	8.796	1.00	41.78
60	ATOM	1467	O	ALA	A	493	33.277	15.410	8.707	1.00	40.76
	ATOM	1468	N	GLY	A	494	34.604	13.960	9.811	1.00	41.01

5	ATOM	1469	CA	GLY	A	494	34.903	14.904	10.873	1.00	41.63
	ATOM	1470	C	GLY	A	494	33.857	15.060	11.965	1.00	41.18
	ATOM	1471	O	GLY	A	494	33.916	16.011	12.747	1.00	38.22
	ATOM	1472	N	LEU	A	495	32.905	14.138	12.043	1.00	39.53
	ATOM	1473	CA	LEU	A	495	31.876	14.248	13.068	1.00	38.91
10	ATOM	1474	CB	LEU	A	495	30.713	13.304	12.769	1.00	39.20
	ATOM	1475	CG	LEU	A	495	29.540	13.901	11.988	1.00	40.73
	ATOM	1476	CD1	LEU	A	495	29.976	14.170	10.553	1.00	37.80
	ATOM	1477	CD2	LEU	A	495	28.349	12.943	12.026	1.00	40.94
	ATOM	1478	C	LEU	A	495	32.461	13.923	14.431	1.00	36.01
15	ATOM	1479	O	LEU	A	495	33.347	13.074	14.544	1.00	34.85
	ATOM	1480	N	THR	A	496	31.979	14.604	15.459	1.00	37.52
	ATOM	1481	CA	THR	A	496	32.462	14.350	16.812	1.00	35.45
	ATOM	1482	CB	THR	A	496	31.925	15.375	17.829	1.00	37.55
	ATOM	1483	OG1	THR	A	496	30.498	15.263	17.908	1.00	32.93
20	ATOM	1484	CG2	THR	A	496	32.315	16.797	17.434	1.00	36.16
	ATOM	1485	C	THR	A	496	31.933	12.987	17.210	1.00	35.67
	ATOM	1486	O	THR	A	496	31.081	12.427	16.521	1.00	34.34
	ATOM	1487	N	LEU	A	497	32.429	12.452	18.319	1.00	34.88
	ATOM	1488	CA	LEU	A	497	31.965	11.151	18.786	1.00	35.67
25	ATOM	1489	CB	LEU	A	497	32.689	10.760	20.074	1.00	41.10
	ATOM	1490	CG	LEU	A	497	33.714	9.640	19.896	1.00	45.27
	ATOM	1491	CD1	LEU	A	497	34.755	9.692	21.008	1.00	45.09
	ATOM	1492	CD2	LEU	A	497	32.988	8.305	19.884	1.00	47.77
	ATOM	1493	C	LEU	A	497	30.455	11.198	19.026	1.00	33.72
30	ATOM	1494	O	LEU	A	497	29.712	10.350	18.534	1.00	33.20
	ATOM	1495	N	GLN	A	498	30.006	12.202	19.773	1.00	30.82
	ATOM	1496	CA	GLN	A	498	28.586	12.348	20.062	1.00	31.47
	ATOM	1497	CB	GLN	A	498	28.344	13.566	20.951	1.00	30.51
	ATOM	1498	CG	GLN	A	498	26.894	13.796	21.341	1.00	34.38
35	ATOM	1499	CD	GLN	A	498	26.712	15.130	22.015	1.00	38.60
	ATOM	1500	OE1	GLN	A	498	27.363	16.112	21.686	1.00	42.92
	ATOM	1501	NE2	GLN	A	498	25.809	15.176	23.008	1.00	40.02
	ATOM	1502	C	GLN	A	498	27.776	12.476	18.773	1.00	30.47
	ATOM	1503	O	GLN	A	498	26.682	11.927	18.665	1.00	30.85
40	ATOM	1504	N	GLN	A	499	28.311	13.196	17.793	1.00	29.52
	ATOM	1505	CA	GLN	A	499	27.603	13.362	16.524	1.00	30.24
	ATOM	1506	CB	GLN	A	499	28.292	14.420	15.661	1.00	30.20
	ATOM	1507	CG	GLN	A	499	28.135	15.840	16.191	1.00	31.60
	ATOM	1508	CD	GLN	A	499	28.930	16.849	15.389	1.00	31.61
45	ATOM	1509	OE1	GLN	A	499	29.956	16.518	14.795	1.00	30.66
	ATOM	1510	NE2	GLN	A	499	28.457	18.089	15.364	1.00	34.17
	ATOM	1511	C	GLN	A	499	27.529	12.047	15.753	1.00	29.40
	ATOM	1512	O	GLN	A	499	26.567	11.793	15.032	1.00	30.04
	ATOM	1513	N	GLN	A	500	28.550	11.214	15.903	1.00	25.67
50	ATOM	1514	CA	GLN	A	500	28.577	9.937	15.216	1.00	29.30
	ATOM	1515	CB	GLN	A	500	29.933	9.276	15.406	1.00	31.52
	ATOM	1516	CG	GLN	A	500	31.012	9.839	14.508	1.00	33.05
	ATOM	1517	CD	GLN	A	500	32.371	9.370	14.930	1.00	34.84
	ATOM	1518	OE1	GLN	A	500	32.612	8.194	15.141	1.00	36.47
55	ATOM	1519	NE2	GLN	A	500	33.301	10.324	15.082	1.00	38.25
	ATOM	1520	C	GLN	A	500	27.459	9.017	15.711	1.00	27.98
	ATOM	1521	O	GLN	A	500	26.700	8.469	14.908	1.00	24.84
	ATOM	1522	N	HIS	A	501	27.357	8.864	17.029	1.00	26.20
	ATOM	1523	CA	HIS	A	501	26.327	8.021	17.631	1.00	27.63
60	ATOM	1524	CB	HIS	A	501	26.535	7.919	19.145	1.00	27.97
	ATOM	1525	CG	HIS	A	501	27.892	7.420	19.535	1.00	34.27

5	ATOM	1526	CD2	HIS	A	501	28.726	6.540	18.931	1.00	36.10
	ATOM	1527	ND1	HIS	A	501	28.541	7.844	20.676	1.00	31.81
	ATOM	1528	CE1	HIS	A	501	29.716	7.244	20.758	1.00	34.89
	ATOM	1529	NE2	HIS	A	501	29.854	6.448	19.712	1.00	37.46
	ATOM	1530	C	HIS	A	501	24.935	8.572	17.348	1.00	24.93
10	ATOM	1531	O	HIS	A	501	23.998	7.815	17.107	1.00	26.73
	ATOM	1532	N	GLN	A	502	24.796	9.892	17.379	1.00	22.79
	ATOM	1533	CA	GLN	A	502	23.504	10.498	17.119	1.00	26.14
	ATOM	1534	CB	GLN	A	502	23.554	12.006	17.371	1.00	22.36
	ATOM	1535	CG	GLN	A	502	23.460	12.378	18.848	1.00	26.19
15	ATOM	1536	CD	GLN	A	502	23.589	13.875	19.089	1.00	28.67
	ATOM	1537	OE1	GLN	A	502	23.632	14.663	18.149	1.00	28.40
	ATOM	1538	NE2	GLN	A	502	23.651	14.268	20.355	1.00	24.72
	ATOM	1539	C	GLN	A	502	23.056	10.221	15.685	1.00	26.19
	ATOM	1540	O	GLN	A	502	21.913	9.822	15.453	1.00	24.09
20	ATOM	1541	N	ARG	A	503	23.955	10.429	14.727	1.00	24.88
	ATOM	1542	CA	ARG	A	503	23.630	10.196	13.326	1.00	25.25
	ATOM	1543	CB	ARG	A	503	24.772	10.668	12.418	1.00	27.63
	ATOM	1544	CG	ARG	A	503	24.432	10.563	10.932	1.00	28.75
	ATOM	1545	CD	ARG	A	503	25.479	11.222	10.056	1.00	27.72
25	ATOM	1546	NE	ARG	A	503	25.072	11.214	8.654	1.00	29.35
	ATOM	1547	CZ	ARG	A	503	24.279	12.126	8.105	1.00	25.84
	ATOM	1548	NH1	ARG	A	503	23.804	13.120	8.840	1.00	27.35
	ATOM	1549	NH2	ARG	A	503	23.962	12.044	6.820	1.00	30.63
	ATOM	1550	C	ARG	A	503	23.347	8.716	13.065	1.00	24.53
30	ATOM	1551	O	ARG	A	503	22.425	8.375	12.321	1.00	25.90
	ATOM	1552	N	LEU	A	504	24.143	7.841	13.672	1.00	23.00
	ATOM	1553	CA	LEU	A	504	23.953	6.406	13.496	1.00	22.60
	ATOM	1554	CB	LEU	A	504	24.971	5.621	14.323	1.00	25.43
	ATOM	1555	CG	LEU	A	504	24.781	4.100	14.344	1.00	25.23
35	ATOM	1556	CD1	LEU	A	504	25.166	3.505	12.991	1.00	28.52
	ATOM	1557	CD2	LEU	A	504	25.627	3.495	15.444	1.00	22.14
	ATOM	1558	C	LEU	A	504	22.541	6.030	13.934	1.00	22.84
	ATOM	1559	O	LEU	A	504	21.846	5.288	13.245	1.00	21.51
	ATOM	1560	N	ALA	A	505	22.120	6.547	15.083	1.00	20.16
40	ATOM	1561	CA	ALA	A	505	20.784	6.262	15.585	1.00	21.08
	ATOM	1562	CB	ALA	A	505	20.605	6.868	16.980	1.00	23.57
	ATOM	1563	C	ALA	A	505	19.738	6.832	14.628	1.00	20.20
	ATOM	1564	O	ALA	A	505	18.754	6.164	14.293	1.00	17.31
	ATOM	1565	N	GLN	A	506	19.954	8.066	14.184	1.00	22.11
45	ATOM	1566	CA	GLN	A	506	19.013	8.711	13.277	1.00	21.70
	ATOM	1567	CB	GLN	A	506	19.502	10.111	12.903	1.00	22.26
	ATOM	1568	CG	GLN	A	506	19.240	11.158	13.975	1.00	25.84
	ATOM	1569	CD	GLN	A	506	20.187	12.333	13.857	1.00	32.88
	ATOM	1570	OE1	GLN	A	506	20.704	12.614	12.777	1.00	31.23
50	ATOM	1571	NE2	GLN	A	506	20.423	13.025	14.968	1.00	32.97
	ATOM	1572	C	GLN	A	506	18.813	7.881	12.016	1.00	23.57
	ATOM	1573	O	GLN	A	506	17.684	7.715	11.550	1.00	21.83
	ATOM	1574	N	LEU	A	507	19.905	7.354	11.474	1.00	19.98
	ATOM	1575	CA	LEU	A	507	19.827	6.537	10.263	1.00	22.03
55	ATOM	1576	CB	LEU	A	507	21.231	6.244	9.725	1.00	23.02
	ATOM	1577	CG	LEU	A	507	22.026	7.457	9.225	1.00	25.80
	ATOM	1578	CD1	LEU	A	507	23.371	6.994	8.713	1.00	27.67
	ATOM	1579	CD2	LEU	A	507	21.264	8.176	8.130	1.00	25.62
	ATOM	1580	C	LEU	A	507	19.090	5.219	10.496	1.00	22.35
60	ATOM	1581	O	LEU	A	507	18.242	4.825	9.695	1.00	19.33
	ATOM	1582	N	LEU	A	508	19.402	4.539	11.592	1.00	21.29

5	ATOM	1583	CA	LEU	A	508	18.755	3.260	11.881	1.00	20.72
	ATOM	1584	CB	LEU	A	508	19.501	2.535	13.001	1.00	22.29
	ATOM	1585	CG	LEU	A	508	20.977	2.311	12.678	1.00	24.70
	ATOM	1586	CD1	LEU	A	508	21.642	1.551	13.814	1.00	21.37
	ATOM	1587	CD2	LEU	A	508	21.095	1.542	11.367	1.00	27.88
10	ATOM	1588	C	LEU	A	508	17.279	3.396	12.239	1.00	19.14
	ATOM	1589	O	LEU	A	508	16.498	2.478	12.003	1.00	17.80
	ATOM	1590	N	LEU	A	509	16.895	4.530	12.815	1.00	19.23
	ATOM	1591	CA	LEU	A	509	15.495	4.747	13.173	1.00	20.14
	ATOM	1592	CB	LEU	A	509	15.347	6.030	13.999	1.00	20.28
15	ATOM	1593	CG	LEU	A	509	15.710	5.858	15.479	1.00	21.35
	ATOM	1594	CD1	LEU	A	509	15.354	7.106	16.263	1.00	19.29
	ATOM	1595	CD2	LEU	A	509	14.989	4.656	16.038	1.00	20.84
	ATOM	1596	C	LEU	A	509	14.681	4.841	11.885	1.00	21.69
	ATOM	1597	O	LEU	A	509	13.493	4.514	11.854	1.00	22.40
20	ATOM	1598	N	ILE	A	510	15.343	5.270	10.815	1.00	20.22
	ATOM	1599	CA	ILE	A	510	14.710	5.397	9.508	1.00	20.40
	ATOM	1600	CB	ILE	A	510	15.720	5.946	8.464	1.00	28.34
	ATOM	1601	CG2	ILE	A	510	15.208	5.710	7.056	1.00	32.54
	ATOM	1602	CG1	ILE	A	510	15.965	7.438	8.696	1.00	28.23
25	ATOM	1603	CD1	ILE	A	510	14.789	8.189	9.288	1.00	33.16
	ATOM	1604	C	ILE	A	510	14.210	4.025	9.049	1.00	23.21
	ATOM	1605	O	ILE	A	510	13.120	3.906	8.474	1.00	21.16
	ATOM	1606	N	LEU	A	511	14.998	2.989	9.323	1.00	18.38
	ATOM	1607	CA	LEU	A	511	14.633	1.634	8.917	1.00	20.10
30	ATOM	1608	CB	LEU	A	511	15.754	0.656	9.267	1.00	21.69
	ATOM	1609	CG	LEU	A	511	17.128	1.022	8.692	1.00	26.03
	ATOM	1610	CD1	LEU	A	511	18.024	-0.206	8.724	1.00	22.68
	ATOM	1611	CD2	LEU	A	511	16.996	1.544	7.267	1.00	26.00
	ATOM	1612	C	LEU	A	511	13.326	1.181	9.543	1.00	18.51
35	ATOM	1613	O	LEU	A	511	12.663	0.283	9.025	1.00	17.40
	ATOM	1614	N	SER	A	512	12.963	1.799	10.664	1.00	18.68
	ATOM	1615	CA	SER	A	512	11.718	1.471	11.331	1.00	18.67
	ATOM	1616	CB	SER	A	512	11.661	2.117	12.720	1.00	18.58
	ATOM	1617	OG	SER	A	512	10.315	2.229	13.165	1.00	27.92
40	ATOM	1618	C	SER	A	512	10.572	1.994	10.464	1.00	18.43
	ATOM	1619	O	SER	A	512	9.584	1.296	10.236	1.00	13.91
	ATOM	1620	N	HIS	A	513	10.713	3.228	9.982	1.00	18.95
	ATOM	1621	CA	HIS	A	513	9.698	3.831	9.124	1.00	20.82
	ATOM	1622	CB	HIS	A	513	10.013	5.315	8.894	1.00	24.36
45	ATOM	1623	CG	HIS	A	513	9.923	6.146	10.136	1.00	32.13
	ATOM	1624	CD2	HIS	A	513	8.863	6.744	10.734	1.00	35.29
	ATOM	1625	ND1	HIS	A	513	11.010	6.391	10.949	1.00	35.00
	ATOM	1626	CE1	HIS	A	513	10.624	7.101	11.995	1.00	34.67
	ATOM	1627	NE2	HIS	A	513	9.326	7.328	11.889	1.00	35.82
50	ATOM	1628	C	HIS	A	513	9.650	3.079	7.790	1.00	19.08
	ATOM	1629	O	HIS	A	513	8.575	2.863	7.220	1.00	21.20
	ATOM	1630	N	ILE	A	514	10.809	2.662	7.297	1.00	15.58
	ATOM	1631	CA	ILE	A	514	10.849	1.921	6.038	1.00	16.48
	ATOM	1632	CB	ILE	A	514	12.312	1.678	5.576	1.00	20.09
55	ATOM	1633	CG2	ILE	A	514	12.349	0.602	4.499	1.00	19.55
	ATOM	1634	CG1	ILE	A	514	12.891	2.986	5.019	1.00	22.62
	ATOM	1635	CD1	ILE	A	514	14.393	2.992	4.874	1.00	27.34
	ATOM	1636	C	ILE	A	514	10.112	0.590	6.210	1.00	16.40
	ATOM	1637	O	ILE	A	514	9.364	0.164	5.328	1.00	17.91
60	ATOM	1638	N	ARG	A	515	10.301	-0.071	7.347	1.00	18.20
	ATOM	1639	CA	ARG	A	515	9.585	-1.327	7.564	1.00	18.05

5	ATOM	1640	CB	ARG	A	515	9.984	-1.980	8.889	1.00	18.36
	ATOM	1641	CG	ARG	A	515	9.173	-3.237	9.213	1.00	17.84
	ATOM	1642	CD	ARG	A	515	9.823	-4.470	8.606	1.00	17.94
	ATOM	1643	NE	ARG	A	515	11.038	-4.813	9.334	1.00	26.96
	ATOM	1644	CZ	ARG	A	515	11.406	-6.051	9.641	1.00	25.13
10	ATOM	1645	NH1	ARG	A	515	10.654	-7.080	9.281	1.00	23.49
	ATOM	1646	NH2	ARG	A	515	12.511	-6.254	10.340	1.00	32.16
	ATOM	1647	C	ARG	A	515	8.089	-1.020	7.594	1.00	18.29
	ATOM	1648	O	ARG	A	515	7.275	-1.759	7.038	1.00	16.22
	ATOM	1649	N	HIS	A	516	7.726	0.085	8.237	1.00	19.33
15	ATOM	1650	CA	HIS	A	516	6.317	0.441	8.330	1.00	17.78
	ATOM	1651	CB	HIS	A	516	6.126	1.702	9.166	1.00	16.84
	ATOM	1652	CG	HIS	A	516	4.692	2.101	9.312	1.00	18.16
	ATOM	1653	CD2	HIS	A	516	3.967	3.061	8.691	1.00	21.17
	ATOM	1654	ND1	HIS	A	516	3.830	1.469	10.180	1.00	20.70
20	ATOM	1655	CE1	HIS	A	516	2.633	2.022	10.089	1.00	21.52
	ATOM	1656	NE2	HIS	A	516	2.689	2.992	9.191	1.00	20.16
	ATOM	1657	C	HIS	A	516	5.708	0.659	6.954	1.00	16.63
	ATOM	1658	O	HIS	A	516	4.598	0.216	6.689	1.00	18.58
	ATOM	1659	N	MET	A	517	6.438	1.334	6.073	1.00	15.29
25	ATOM	1660	CA	MET	A	517	5.925	1.589	4.730	1.00	16.58
	ATOM	1661	CB	MET	A	517	6.837	2.576	4.002	1.00	18.66
	ATOM	1662	CG	MET	A	517	6.805	3.978	4.631	1.00	16.88
	ATOM	1663	SD	MET	A	517	7.670	5.243	3.701	1.00	24.08
	ATOM	1664	CE	MET	A	517	9.390	4.777	3.962	1.00	14.30
30	ATOM	1665	C	MET	A	517	5.773	0.289	3.940	1.00	17.86
	ATOM	1666	O	MET	A	517	4.791	0.101	3.224	1.00	18.25
	ATOM	1667	N	SER	A	518	6.741	-0.610	4.086	1.00	17.43
	ATOM	1668	CA	SER	A	518	6.697	-1.896	3.403	1.00	18.40
	ATOM	1669	CB	SER	A	518	7.974	-2.695	3.680	1.00	16.77
35	ATOM	1670	OG	SER	A	518	7.834	-4.030	3.227	1.00	24.23
	ATOM	1671	C	SER	A	518	5.476	-2.695	3.854	1.00	17.91
	ATOM	1672	O	SER	A	518	4.788	-3.295	3.030	1.00	18.97
	ATOM	1673	N	ASN	A	519	5.204	-2.697	5.159	1.00	21.82
	ATOM	1674	CA	ASN	A	519	4.047	-3.418	5.696	1.00	21.99
40	ATOM	1675	CB	ASN	A	519	3.957	-3.257	7.216	1.00	23.24
	ATOM	1676	CG	ASN	A	519	5.046	-4.011	7.957	1.00	31.14
	ATOM	1677	OD1	ASN	A	519	5.585	-4.999	7.461	1.00	32.50
	ATOM	1678	ND2	ASN	A	519	5.368	-3.545	9.163	1.00	29.10
	ATOM	1679	C	ASN	A	519	2.761	-2.871	5.079	1.00	23.76
45	ATOM	1680	O	ASN	A	519	1.902	-3.632	4.631	1.00	24.48
	ATOM	1681	N	LYS	A	520	2.627	-1.548	5.078	1.00	20.58
	ATOM	1682	CA	LYS	A	520	1.449	-0.900	4.512	1.00	25.49
	ATOM	1683	CB	LYS	A	520	1.484	0.607	4.786	1.00	24.73
	ATOM	1684	CG	LYS	A	520	1.512	0.996	6.264	1.00	32.31
50	ATOM	1685	CD	LYS	A	520	0.656	0.080	7.133	1.00	37.11
	ATOM	1686	CE	LYS	A	520	-0.787	0.547	7.181	1.00	41.56
	ATOM	1687	NZ	LYS	A	520	-1.560	-0.134	8.261	1.00	42.66
	ATOM	1688	C	LYS	A	520	1.380	-1.144	3.005	1.00	25.40
	ATOM	1689	O	LYS	A	520	0.316	-1.436	2.467	1.00	26.44
55	ATOM	1690	N	GLY	A	521	2.520	-1.021	2.332	1.00	22.88
	ATOM	1691	CA	GLY	A	521	2.561	-1.236	0.897	1.00	21.53
	ATOM	1692	C	GLY	A	521	2.177	-2.655	0.536	1.00	24.79
	ATOM	1693	O	GLY	A	521	1.426	-2.878	-0.413	1.00	25.71
	ATOM	1694	N	MET	A	522	2.696	-3.619	1.290	1.00	22.75
60	ATOM	1695	CA	MET	A	522	2.393	-5.027	1.058	1.00	23.40
	ATOM	1696	CB	MET	A	522	3.170	-5.898	2.042	1.00	25.74

5	ATOM	1697	CG	MET	A	522	3.396	-7.308	1.559	1.00	31.06
	ATOM	1698	SD	MET	A	522	4.572	-7.352	0.202	1.00	34.06
	ATOM	1699	CE	MET	A	522	6.125	-7.229	1.113	1.00	29.28
	ATOM	1700	C	MET	A	522	0.893	-5.281	1.218	1.00	26.49
	ATOM	1701	O	MET	A	522	0.268	-5.920	0.361	1.00	25.47
10	ATOM	1702	N	GLU	A	523	0.321	-4.790	2.318	1.00	24.95
	ATOM	1703	CA	GLU	A	523	-1.110	-4.954	2.566	1.00	27.15
	ATOM	1704	CB	GLU	A	523	-1.555	-4.206	3.835	1.00	31.08
	ATOM	1705	CG	GLU	A	523	-0.830	-4.564	5.124	1.00	38.93
	ATOM	1706	CD	GLU	A	523	-1.153	-3.585	6.258	1.00	46.90
15	ATOM	1707	OE1	GLU	A	523	-2.225	-2.938	6.200	1.00	47.40
	ATOM	1708	OE2	GLU	A	523	-0.337	-3.460	7.202	1.00	47.39
	ATOM	1709	C	GLU	A	523	-1.872	-4.368	1.381	1.00	26.10
	ATOM	1710	O	GLU	A	523	-2.817	-4.964	0.882	1.00	24.25
	ATOM	1711	N	HIS	A	524	-1.449	-3.182	0.940	1.00	24.74
20	ATOM	1712	CA	HIS	A	524	-2.093	-2.505	-0.173	1.00	26.17
	ATOM	1713	CB	HIS	A	524	-1.481	-1.125	-0.379	1.00	24.64
	ATOM	1714	CG	HIS	A	524	-2.233	-0.278	-1.355	1.00	30.59
	ATOM	1715	CD2	HIS	A	524	-3.227	0.624	-1.172	1.00	32.15
	ATOM	1716	ND1	HIS	A	524	-2.008	-0.332	-2.713	1.00	27.46
25	ATOM	1717	CE1	HIS	A	524	-2.829	0.502	-3.326	1.00	34.58
	ATOM	1718	NE2	HIS	A	524	-3.580	1.094	-2.413	1.00	30.50
	ATOM	1719	C	HIS	A	524	-1.996	-3.294	-1.474	1.00	28.06
	ATOM	1720	O	HIS	A	524	-2.976	-3.419	-2.217	1.00	29.81
	ATOM	1721	N	LEU	A	525	-0.811	-3.824	-1.746	1.00	27.07
30	ATOM	1722	CA	LEU	A	525	-0.594	-4.601	-2.955	1.00	29.30
	ATOM	1723	CB	LEU	A	525	0.865	-5.039	-3.051	1.00	26.39
	ATOM	1724	CG	LEU	A	525	1.307	-5.765	-4.321	1.00	29.34
	ATOM	1725	CD1	LEU	A	525	0.734	-5.076	-5.562	1.00	29.61
	ATOM	1726	CD2	LEU	A	525	2.829	-5.769	-4.370	1.00	29.22
35	ATOM	1727	C	LEU	A	525	-1.497	-5.822	-2.950	1.00	31.67
	ATOM	1728	O	LEU	A	525	-2.128	-6.133	-3.957	1.00	32.45
	ATOM	1729	N	TYR	A	526	-1.559	-6.512	-1.814	1.00	36.14
	ATOM	1730	CA	TYR	A	526	-2.397	-7.698	-1.696	1.00	40.36
	ATOM	1731	CB	TYR	A	526	-2.221	-8.350	-0.324	1.00	45.27
40	ATOM	1732	CG	TYR	A	526	-2.849	-9.722	-0.229	1.00	50.62
	ATOM	1733	CD1	TYR	A	526	-2.114	-10.867	-0.537	1.00	54.55
	ATOM	1734	CE1	TYR	A	526	-2.698	-12.136	-0.482	1.00	57.27
	ATOM	1735	CD2	TYR	A	526	-4.188	-9.876	0.142	1.00	53.48
	ATOM	1736	CE2	TYR	A	526	-4.781	-11.141	0.201	1.00	55.93
45	ATOM	1737	CZ	TYR	A	526	-4.029	-12.264	-0.113	1.00	56.60
	ATOM	1738	OH	TYR	A	526	-4.603	-13.515	-0.063	1.00	60.70
	ATOM	1739	C	TYR	A	526	-3.852	-7.298	-1.893	1.00	42.83
	ATOM	1740	O	TYR	A	526	-4.673	-8.094	-2.349	1.00	43.49
	ATOM	1741	N	SER	A	527	-4.158	-6.055	-1.543	1.00	41.55
50	ATOM	1742	CA	SER	A	527	-5.503	-5.523	-1.686	1.00	44.04
	ATOM	1743	CB	SER	A	527	-5.606	-4.169	-0.979	1.00	43.47
	ATOM	1744	OG	SER	A	527	-6.954	-3.789	-0.786	1.00	47.51
	ATOM	1745	C	SER	A	527	-5.817	-5.356	-3.172	1.00	44.18
	ATOM	1746	O	SER	A	527	-6.883	-5.757	-3.642	1.00	44.88
55	ATOM	1747	N	MET	A	528	-4.883	-4.755	-3.901	1.00	41.79
	ATOM	1748	CA	MET	A	528	-5.047	-4.536	-5.331	1.00	44.04
	ATOM	1749	CB	MET	A	528	-3.898	-3.679	-5.870	1.00	44.78
	ATOM	1750	CG	MET	A	528	-3.965	-2.206	-5.468	1.00	45.37
	ATOM	1751	SD	MET	A	528	-5.652	-1.598	-5.273	1.00	51.83
60	ATOM	1752	CE	MET	A	528	-5.553	-0.004	-6.044	1.00	46.61
	ATOM	1753	C	MET	A	528	-5.087	-5.871	-6.071	1.00	44.29

5	ATOM	1754	O	MET	A	528	-5.689	-5.979	-7.137	1.00	44.02
	ATOM	1755	N	LYS	A	529	-4.443	-6.883	-5.499	1.00	46.78
	ATOM	1756	CA	LYS	A	529	-4.413	-8.213	-6.099	1.00	51.28
	ATOM	1757	CB	LYS	A	529	-3.550	-9.158	-5.261	1.00	50.87
	ATOM	1758	CG	LYS	A	529	-2.798	-10.204	-6.071	1.00	50.55
10	ATOM	1759	CD	LYS	A	529	-3.548	-11.520	-6.104	1.00	51.25
	ATOM	1760	CE	LYS	A	529	-2.616	-12.694	-5.856	1.00	53.22
	ATOM	1761	NZ	LYS	A	529	-2.420	-12.954	-4.402	1.00	53.22
	ATOM	1762	C	LYS	A	529	-5.829	-8.768	-6.182	1.00	54.27
	ATOM	1763	O	LYS	A	529	-6.325	-9.069	-7.266	1.00	55.50
15	ATOM	1764	N	CYS	A	530	-6.472	-8.901	-5.027	1.00	56.71
	ATOM	1765	CA	CYS	A	530	-7.833	-9.416	-4.961	1.00	58.35
	ATOM	1766	CB	CYS	A	530	-8.333	-9.380	-3.517	1.00	59.78
	ATOM	1767	SG	CYS	A	530	-7.289	-10.304	-2.358	1.00	63.19
	ATOM	1768	C	CYS	A	530	-8.766	-8.609	-5.858	1.00	59.36
20	ATOM	1769	O	CYS	A	530	-9.644	-9.169	-6.514	1.00	59.52
	ATOM	1770	N	LYS	A	531	-8.569	-7.293	-5.888	1.00	59.24
	ATOM	1771	CA	LYS	A	531	-9.390	-6.411	-6.713	1.00	60.14
	ATOM	1772	CB	LYS	A	531	-9.158	-4.952	-6.317	1.00	58.92
	ATOM	1773	C	LYS	A	531	-9.073	-6.615	-8.195	1.00	61.48
25	ATOM	1774	O	LYS	A	531	-9.618	-5.928	-9.061	1.00	61.74
	ATOM	1775	N	ASN	A	532	-8.179	-7.561	-8.474	1.00	61.65
	ATOM	1776	CA	ASN	A	532	-7.783	-7.890	-9.840	1.00	61.60
	ATOM	1777	CB	ASN	A	532	-8.966	-8.518	-10.581	1.00	62.28
	ATOM	1778	CG	ASN	A	532	-8.750	-9.985	-10.878	1.00	64.66
30	ATOM	1779	OD1	ASN	A	532	-8.344	-10.352	-11.983	1.00	67.08
	ATOM	1780	ND2	ASN	A	532	-9.016	-10.836	-9.891	1.00	62.68
	ATOM	1781	C	ASN	A	532	-7.247	-6.710	-10.648	1.00	59.75
	ATOM	1782	O	ASN	A	532	-7.487	-6.615	-11.850	1.00	57.50
	ATOM	1783	N	VAL	A	533	-6.507	-5.822	-9.992	1.00	59.39
35	ATOM	1784	CA	VAL	A	533	-5.954	-4.656	-10.669	1.00	58.22
	ATOM	1785	CB	VAL	A	533	-6.223	-3.371	-9.865	1.00	59.20
	ATOM	1786	CG1	VAL	A	533	-6.181	-2.163	-10.785	1.00	59.21
	ATOM	1787	CG2	VAL	A	533	-7.574	-3.467	-9.172	1.00	59.57
	ATOM	1788	C	VAL	A	533	-4.452	-4.767	-10.907	1.00	57.86
40	ATOM	1789	O	VAL	A	533	-3.846	-3.874	-11.499	1.00	60.56
	ATOM	1790	N	VAL	A	534	-3.852	-5.863	-10.451	1.00	56.03
	ATOM	1791	CA	VAL	A	534	-2.417	-6.063	-10.621	1.00	54.11
	ATOM	1792	CB	VAL	A	534	-1.767	-6.632	-9.341	1.00	54.02
	ATOM	1793	CG1	VAL	A	534	-0.300	-6.950	-9.601	1.00	52.37
45	ATOM	1794	CG2	VAL	A	534	-1.900	-5.635	-8.200	1.00	55.70
	ATOM	1795	C	VAL	A	534	-2.089	-7.008	-11.770	1.00	54.31
	ATOM	1796	O	VAL	A	534	-2.519	-8.164	-11.780	1.00	51.66
	ATOM	1797	N	PRO	A	535	-1.315	-6.527	-12.755	1.00	53.54
	ATOM	1798	CD	PRO	A	535	-0.749	-5.172	-12.874	1.00	54.28
50	ATOM	1799	CA	PRO	A	535	-0.949	-7.373	-13.893	1.00	53.24
	ATOM	1800	CB	PRO	A	535	0.011	-6.500	-14.697	1.00	52.71
	ATOM	1801	CG	PRO	A	535	-0.353	-5.102	-14.319	1.00	53.19
	ATOM	1802	C	PRO	A	535	-0.296	-8.664	-13.411	1.00	54.25
	ATOM	1803	O	PRO	A	535	0.121	-8.768	-12.254	1.00	54.56
55	ATOM	1804	N	LEU	A	536	-0.203	-9.645	-14.299	1.00	53.63
	ATOM	1805	CA	LEU	A	536	0.382	-10.926	-13.937	1.00	53.11
	ATOM	1806	CB	LEU	A	536	-0.250	-12.046	-14.763	1.00	51.88
	ATOM	1807	CG	LEU	A	536	-0.686	-13.256	-13.938	1.00	51.83
	ATOM	1808	CD1	LEU	A	536	-1.953	-12.917	-13.173	1.00	49.51
60	ATOM	1809	CD2	LEU	A	536	-0.905	-14.449	-14.854	1.00	53.43
	ATOM	1810	C	LEU	A	536	1.895	-10.990	-14.081	1.00	52.58

5	ATOM	1811	O	LEU	A	536	2.414	-11.501	-15.075	1.00	55.33
	ATOM	1812	N	TYR	A	537	2.601	-10.462	-13.087	1.00	48.72
	ATOM	1813	CA	TYR	A	537	4.057	-10.501	-13.093	1.00	44.22
	ATOM	1814	CB	TYR	A	537	4.627	-9.134	-12.709	1.00	44.52
	ATOM	1815	CG	TYR	A	537	4.331	-8.053	-13.731	1.00	45.18
10	ATOM	1816	CD1	TYR	A	537	3.623	-6.905	-13.376	1.00	43.77
	ATOM	1817	CE1	TYR	A	537	3.334	-5.915	-14.317	1.00	45.23
	ATOM	1818	CD2	TYR	A	537	4.747	-8.187	-15.058	1.00	46.91
	ATOM	1819	CE2	TYR	A	537	4.462	-7.202	-16.008	1.00	43.93
	ATOM	1820	CZ	TYR	A	537	3.757	-6.071	-15.631	1.00	46.70
15	ATOM	1821	OH	TYR	A	537	3.472	-5.097	-16.565	1.00	48.35
	ATOM	1822	C	TYR	A	537	4.401	-11.562	-12.056	1.00	41.29
	ATOM	1823	O	TYR	A	537	4.330	-11.319	-10.856	1.00	41.82
	ATOM	1824	N	ASP	A	538	4.748	-12.748	-12.540	1.00	40.34
	ATOM	1825	CA	ASP	A	538	5.055	-13.896	-11.691	1.00	38.84
20	ATOM	1826	CB	ASP	A	538	5.594	-15.037	-12.554	1.00	43.47
	ATOM	1827	CG	ASP	A	538	4.571	-15.531	-13.566	1.00	47.67
	ATOM	1828	OD1	ASP	A	538	4.931	-16.373	-14.416	1.00	49.33
	ATOM	1829	OD2	ASP	A	538	3.405	-15.073	-13.511	1.00	48.07
	ATOM	1830	C	ASP	A	538	5.991	-13.676	-10.508	1.00	37.28
25	ATOM	1831	O	ASP	A	538	5.620	-13.964	-9.371	1.00	38.55
	ATOM	1832	N	LEU	A	539	7.196	-13.200	-10.766	1.00	33.83
	ATOM	1833	CA	LEU	A	539	8.155	-12.959	-9.692	1.00	32.80
	ATOM	1834	CB	LEU	A	539	9.419	-12.323	-10.263	1.00	32.78
	ATOM	1835	CG	LEU	A	539	10.561	-12.031	-9.292	1.00	30.93
30	ATOM	1836	CD1	LEU	A	539	10.913	-13.280	-8.492	1.00	33.81
	ATOM	1837	CD2	LEU	A	539	11.758	-11.538	-10.077	1.00	25.92
	ATOM	1838	C	LEU	A	539	7.558	-12.050	-8.614	1.00	31.85
	ATOM	1839	O	LEU	A	539	7.590	-12.367	-7.423	1.00	25.63
	ATOM	1840	N	LEU	A	540	7.011	-10.917	-9.042	1.00	32.07
35	ATOM	1841	CA	LEU	A	540	6.411	-9.976	-8.111	1.00	31.03
	ATOM	1842	CB	LEU	A	540	5.792	-8.800	-8.861	1.00	30.56
	ATOM	1843	CG	LEU	A	540	5.124	-7.774	-7.945	1.00	31.12
	ATOM	1844	CD1	LEU	A	540	6.092	-7.357	-6.838	1.00	29.76
	ATOM	1845	CD2	LEU	A	540	4.693	-6.572	-8.762	1.00	30.85
40	ATOM	1846	C	LEU	A	540	5.337	-10.660	-7.282	1.00	34.55
	ATOM	1847	O	LEU	A	540	5.316	-10.522	-6.063	1.00	31.60
	ATOM	1848	N	LEU	A	541	4.446	-11.388	-7.941	1.00	35.64
	ATOM	1849	CA	LEU	A	541	3.378	-12.101	-7.245	1.00	37.84
	ATOM	1850	CB	LEU	A	541	2.452	-12.771	-8.255	1.00	38.49
45	ATOM	1851	CG	LEU	A	541	1.244	-11.932	-8.678	1.00	39.80
	ATOM	1852	CD1	LEU	A	541	0.476	-11.476	-7.448	1.00	40.02
	ATOM	1853	CD2	LEU	A	541	1.713	-10.733	-9.485	1.00	40.48
	ATOM	1854	C	LEU	A	541	3.937	-13.147	-6.275	1.00	40.10
	ATOM	1855	O	LEU	A	541	3.472	-13.254	-5.137	1.00	42.72
50	ATOM	1856	N	GLU	A	542	4.929	-13.915	-6.723	1.00	38.45
	ATOM	1857	CA	GLU	A	542	5.535	-14.932	-5.868	1.00	39.59
	ATOM	1858	CB	GLU	A	542	6.738	-15.566	-6.564	1.00	41.73
	ATOM	1859	CG	GLU	A	542	6.396	-16.327	-7.831	1.00	48.34
	ATOM	1860	CD	GLU	A	542	6.931	-17.747	-7.819	1.00	52.57
55	ATOM	1861	OE1	GLU	A	542	8.049	-17.961	-7.298	1.00	52.70
	ATOM	1862	OE2	GLU	A	542	6.230	-18.647	-8.331	1.00	53.69
	ATOM	1863	C	GLU	A	542	5.989	-14.299	-4.553	1.00	39.94
	ATOM	1864	O	GLU	A	542	5.567	-14.710	-3.472	1.00	40.99
	ATOM	1865	N	MET	A	543	6.844	-13.287	-4.663	1.00	38.29
60	ATOM	1866	CA	MET	A	543	7.380	-12.580	-3.503	1.00	38.11
	ATOM	1867	CB	MET	A	543	8.242	-11.408	-3.963	1.00	37.34



5	ATOM	1868	CG	MET	A	543	9.311	-11.797	-4.953	1.00	40.59
	ATOM	1869	SD	MET	A	543	10.829	-12.223	-4.114	1.00	45.64
	ATOM	1870	CE	MET	A	543	12.014	-11.399	-5.151	1.00	42.61
	ATOM	1871	C	MET	A	543	6.287	-12.064	-2.581	1.00	37.94
	ATOM	1872	O	MET	A	543	6.413	-12.127	-1.358	1.00	39.20
10	ATOM	1873	N	LEU	A	544	5.218	-11.544	-3.175	1.00	39.44
	ATOM	1874	CA	LEU	A	544	4.100	-11.013	-2.408	1.00	40.91
	ATOM	1875	CB	LEU	A	544	3.087	-10.344	-3.341	1.00	39.88
	ATOM	1876	CG	LEU	A	544	1.775	-9.905	-2.688	1.00	42.70
	ATOM	1877	CD1	LEU	A	544	2.060	-8.886	-1.586	1.00	37.35
15	ATOM	1878	CD2	LEU	A	544	0.854	-9.317	-3.741	1.00	38.47
	ATOM	1879	C	LEU	A	544	3.420	-12.120	-1.614	1.00	42.83
	ATOM	1880	O	LEU	A	544	2.957	-11.899	-0.496	1.00	42.73
	ATOM	1881	N	ASP	A	545	3.367	-13.313	-2.197	1.00	46.32
	ATOM	1882	CA	ASP	A	545	2.746	-14.456	-1.539	1.00	50.65
20	ATOM	1883	CB	ASP	A	545	2.606	-15.617	-2.524	1.00	53.67
	ATOM	1884	CG	ASP	A	545	1.703	-15.278	-3.691	1.00	57.35
	ATOM	1885	OD1	ASP	A	545	0.697	-14.568	-3.475	1.00	59.99
	ATOM	1886	OD2	ASP	A	545	1.999	-15.718	-4.824	1.00	59.68
	ATOM	1887	C	ASP	A	545	3.559	-14.898	-0.327	1.00	50.74
25	ATOM	1888	O	ASP	A	545	3.004	-15.388	0.657	1.00	49.39
	ATOM	1889	N	ALA	A	546	4.874	-14.723	-0.401	1.00	51.82
	ATOM	1890	CA	ALA	A	546	5.750	-15.095	0.702	1.00	53.12
	ATOM	1891	CB	ALA	A	546	7.180	-14.678	0.395	1.00	53.19
	ATOM	1892	C	ALA	A	546	5.269	-14.424	1.987	1.00	54.67
30	ATOM	1893	O	ALA	A	546	5.476	-14.940	3.085	1.00	52.32
	ATOM	1894	N	HIS	A	547	4.622	-13.270	1.838	1.00	56.66
	ATOM	1895	CA	HIS	A	547	4.102	-12.520	2.978	1.00	59.19
	ATOM	1896	CB	HIS	A	547	4.144	-11.017	2.684	1.00	56.70
	ATOM	1897	CG	HIS	A	547	5.489	-10.394	2.896	1.00	54.64
35	ATOM	1898	CD2	HIS	A	547	6.644	-10.506	2.199	1.00	53.92
	ATOM	1899	ND1	HIS	A	547	5.748	-9.514	3.925	1.00	52.17
	ATOM	1900	CE1	HIS	A	547	7.004	-9.111	3.853	1.00	52.16
	ATOM	1901	NE2	HIS	A	547	7.570	-9.698	2.814	1.00	51.90
	ATOM	1902	C	HIS	A	547	2.668	-12.940	3.306	1.00	62.77
40	ATOM	1903	O	HIS	A	547	1.842	-12.120	3.707	1.00	63.24
	ATOM	1904	N	ARG	A	548	2.381	-14.224	3.133	1.00	68.37
	ATOM	1905	CA	ARG	A	548	1.053	-14.758	3.411	1.00	72.75
	ATOM	1906	CB	ARG	A	548	0.243	-14.864	2.113	1.00	73.73
	ATOM	1907	CG	ARG	A	548	-1.149	-14.243	2.186	1.00	74.04
45	ATOM	1908	CD	ARG	A	548	-1.081	-12.728	2.297	1.00	74.50
	ATOM	1909	NE	ARG	A	548	-2.305	-12.167	2.863	1.00	75.04
	ATOM	1910	CZ	ARG	A	548	-2.478	-10.880	3.149	1.00	75.59
	ATOM	1911	NH1	ARG	A	548	-1.506	-10.006	2.919	1.00	75.79
	ATOM	1912	NH2	ARG	A	548	-3.627	-10.464	3.662	1.00	76.00
50	ATOM	1913	C	ARG	A	548	1.179	-16.133	4.061	1.00	74.94
	ATOM	1914	O	ARG	A	548	0.197	-16.697	4.549	1.00	75.15
	ATOM	1915	N	LEU	A	549	2.398	-16.665	4.063	1.00	76.49
	ATOM	1916	CA	LEU	A	549	2.669	-17.969	4.653	1.00	78.14
	ATOM	1917	CB	LEU	A	549	2.971	-18.986	3.557	1.00	77.55
55	ATOM	1918	C	LEU	A	549	3.846	-17.870	5.619	1.00	79.13
	ATOM	1919	O	LEU	A	549	4.892	-17.317	5.215	1.00	80.40
	ATOM	1920	OXT	LEU	A	549	3.708	-18.341	6.769	1.00	79.46
	HETATM	1921	CP9	DES	A	600	5.390	-3.061	-6.139	1.00	21.38
	HETATM	1922	CP8	DES	A	600	5.834	-1.989	-5.134	1.00	22.41
60	HETATM	1923	CP7	DES	A	600	5.038	-0.714	-5.236	1.00	21.32
	HETATM	1924	CP6	DES	A	600	3.587	-0.864	-5.062	1.00	25.87

5	HETATM	1925	CP1	DES	A	600	2.987	-0.978	-3.784	1.00	23.92
	HETATM	1926	CP2	DES	A	600	1.597	-1.150	-3.684	1.00	29.77
	HETATM	1927	CP3	DES	A	600	0.842	-1.214	-4.871	1.00	31.40
	HETATM	1928	OP3	DES	A	600	-0.506	-1.419	-4.824	1.00	33.36
10	HETATM	1929	CP4	DES	A	600	1.421	-1.099	-6.143	1.00	27.01
	HETATM	1930	CP5	DES	A	600	2.793	-0.929	-6.230	1.00	27.40
	HETATM	1931	C7	DES	A	600	5.671	0.461	-5.482	1.00	22.39
	HETATM	1932	C6	DES	A	600	7.113	0.561	-5.809	1.00	21.75
15	HETATM	1933	C5	DES	A	600	7.541	0.306	-7.131	1.00	19.97
	HETATM	1934	C4	DES	A	600	8.889	0.429	-7.477	1.00	23.81
	HETATM	1935	C3	DES	A	600	9.814	0.804	-6.488	1.00	21.88
	HETATM	1936	O3	DES	A	600	11.125	0.901	-6.839	1.00	22.32
20	HETATM	1937	C2	DES	A	600	9.423	1.066	-5.161	1.00	19.74
	HETATM	1938	C1	DES	A	600	8.066	0.937	-4.838	1.00	21.25
	HETATM	1939	C8	DES	A	600	4.894	1.765	-5.443	1.00	21.47
	HETATM	1940	C9	DES	A	600	4.959	2.468	-4.070	1.00	21.38
25	HETATM	1941	CL	CL	A	601	14.781	-3.035	-17.739	1.00	24.10
	ATOM	1942	CB	SER	B	305	12.321	21.086	25.295	1.00	64.27
	ATOM	1943	C	SER	B	305	12.672	22.102	27.548	1.00	64.37
	ATOM	1944	O	SER	B	305	13.701	22.760	27.702	1.00	66.90
30	ATOM	1945	N	SER	B	305	12.045	23.521	25.606	1.00	63.72
	ATOM	1946	CA	SER	B	305	11.875	22.187	26.251	1.00	64.21
	ATOM	1947	N	LEU	B	306	12.193	21.293	28.484	1.00	63.09
	ATOM	1948	CA	LEU	B	306	12.884	21.133	29.757	1.00	60.98
35	ATOM	1949	CB	LEU	B	306	11.884	21.200	30.913	1.00	61.23
	ATOM	1950	CG	LEU	B	306	12.221	20.417	32.183	1.00	62.23
	ATOM	1951	CD1	LEU	B	306	13.304	21.144	32.966	1.00	62.56
	ATOM	1952	CD2	LEU	B	306	10.965	20.258	33.027	1.00	64.31
40	ATOM	1953	C	LEU	B	306	13.660	19.819	29.803	1.00	58.39
	ATOM	1954	O	LEU	B	306	14.570	19.654	30.614	1.00	58.56
	ATOM	1955	N	ALA	B	307	13.293	18.881	28.933	1.00	54.82
	ATOM	1956	CA	ALA	B	307	13.971	17.589	28.861	1.00	50.62
45	ATOM	1957	CB	ALA	B	307	13.092	16.584	28.143	1.00	51.30
	ATOM	1958	C	ALA	B	307	15.303	17.719	28.122	1.00	46.84
	ATOM	1959	O	ALA	B	307	16.196	16.885	28.274	1.00	45.62
	ATOM	1960	N	LEU	B	308	15.431	18.769	27.320	1.00	43.46
50	ATOM	1961	CA	LEU	B	308	16.643	18.983	26.542	1.00	43.01
	ATOM	1962	CB	LEU	B	308	16.413	20.100	25.526	1.00	41.32
	ATOM	1963	CG	LEU	B	308	16.315	19.708	24.051	1.00	43.10
	ATOM	1964	CD1	LEU	B	308	15.942	18.239	23.903	1.00	40.51
55	ATOM	1965	CD2	LEU	B	308	15.287	20.602	23.375	1.00	39.80
	ATOM	1966	C	LEU	B	308	17.874	19.297	27.385	1.00	42.11
	ATOM	1967	O	LEU	B	308	19.000	19.102	26.932	1.00	44.34
	ATOM	1968	N	SER	B	309	17.669	19.775	28.608	1.00	40.88
60	ATOM	1969	CA	SER	B	309	18.796	20.100	29.475	1.00	42.79
	ATOM	1970	CB	SER	B	309	18.562	21.447	30.163	1.00	41.25
	ATOM	1971	OG	SER	B	309	17.459	21.379	31.046	1.00	46.67
	ATOM	1972	C	SER	B	309	19.072	19.028	30.529	1.00	42.60
65	ATOM	1973	O	SER	B	309	20.053	19.119	31.269	1.00	44.18
	ATOM	1974	N	LEU	B	310	18.217	18.012	30.596	1.00	39.44
	ATOM	1975	CA	LEU	B	310	18.394	16.936	31.569	1.00	37.62
	ATOM	1976	CB	LEU	B	310	17.205	15.969	31.499	1.00	38.84
70	ATOM	1977	CG	LEU	B	310	16.216	15.873	32.668	1.00	42.43
	ATOM	1978	CD1	LEU	B	310	16.040	17.219	33.355	1.00	42.55
	ATOM	1979	CD2	LEU	B	310	14.881	15.380	32.138	1.00	39.69
	ATOM	1980	C	LEU	B	310	19.691	16.174	31.285	1.00	34.11
75	ATOM	1981	O	LEU	B	310	20.111	16.070	30.139	1.00	34.41

5	ATOM	1982	N	THR	B	311	20.339	15.662	32.326	1.00	34.04
	ATOM	1983	CA	THR	B	311	21.564	14.888	32.127	1.00	32.34
	ATOM	1984	CB	THR	B	311	22.434	14.824	33.399	1.00	31.75
	ATOM	1985	OG1	THR	B	311	21.724	14.116	34.420	1.00	36.20
	ATOM	1986	CG2	THR	B	311	22.782	16.212	33.893	1.00	31.05
10	ATOM	1987	C	THR	B	311	21.145	13.460	31.790	1.00	32.37
	ATOM	1988	O	THR	B	311	19.967	13.117	31.899	1.00	28.16
	ATOM	1989	N	ALA	B	312	22.106	12.628	31.396	1.00	33.23
	ATOM	1990	CA	ALA	B	312	21.811	11.237	31.053	1.00	35.63
	ATOM	1991	CB	ALA	B	312	23.077	10.527	30.577	1.00	34.00
15	ATOM	1992	C	ALA	B	312	21.210	10.489	32.240	1.00	34.29
	ATOM	1993	O	ALA	B	312	20.226	9.766	32.089	1.00	33.10
	ATOM	1994	N	ASP	B	313	21.800	10.665	33.419	1.00	33.90
	ATOM	1995	CA	ASP	B	313	21.304	9.994	34.615	1.00	34.19
	ATOM	1996	CB	ASP	B	313	22.258	10.219	35.788	1.00	42.09
20	ATOM	1997	CG	ASP	B	313	23.494	9.358	35.700	1.00	44.87
	ATOM	1998	OD1	ASP	B	313	24.586	9.858	36.040	1.00	51.57
	ATOM	1999	OD2	ASP	B	313	23.377	8.184	35.290	1.00	46.79
	ATOM	2000	C	ASP	B	313	19.925	10.520	34.971	1.00	31.99
	ATOM	2001	O	ASP	B	313	19.056	9.768	35.426	1.00	32.03
25	ATOM	2002	N	GLN	B	314	19.733	11.819	34.763	1.00	29.38
	ATOM	2003	CA	GLN	B	314	18.458	12.457	35.046	1.00	29.73
	ATOM	2004	CB	GLN	B	314	18.562	13.966	34.832	1.00	32.88
	ATOM	2005	CG	GLN	B	314	18.970	14.732	36.085	1.00	36.47
	ATOM	2006	CD	GLN	B	314	19.213	16.208	35.815	1.00	36.76
30	ATOM	2007	OE1	GLN	B	314	19.300	16.634	34.664	1.00	38.79
	ATOM	2008	NE2	GLN	B	314	19.327	16.995	36.880	1.00	39.72
	ATOM	2009	C	GLN	B	314	17.409	11.873	34.116	1.00	29.11
	ATOM	2010	O	GLN	B	314	16.274	11.620	34.522	1.00	28.82
	ATOM	2011	N	MET	B	315	17.801	11.657	32.864	1.00	27.27
35	ATOM	2012	CA	MET	B	315	16.900	11.079	31.872	1.00	30.41
	ATOM	2013	CB	MET	B	315	17.595	11.029	30.509	1.00	30.10
	ATOM	2014	CG	MET	B	315	16.787	10.345	29.421	1.00	38.02
	ATOM	2015	SD	MET	B	315	15.252	11.220	29.065	1.00	41.12
	ATOM	2016	CE	MET	B	315	15.890	12.835	28.611	1.00	39.32
40	ATOM	2017	C	MET	B	315	16.490	9.665	32.311	1.00	27.99
	ATOM	2018	O	MET	B	315	15.302	9.351	32.396	1.00	26.60
	ATOM	2019	N	VAL	B	316	17.481	8.823	32.598	1.00	27.26
	ATOM	2020	CA	VAL	B	316	17.229	7.447	33.027	1.00	24.54
	ATOM	2021	CB	VAL	B	316	18.554	6.708	33.351	1.00	26.22
45	ATOM	2022	CG1	VAL	B	316	18.272	5.404	34.096	1.00	29.81
	ATOM	2023	CG2	VAL	B	316	19.302	6.410	32.074	1.00	29.75
	ATOM	2024	C	VAL	B	316	16.326	7.389	34.258	1.00	27.22
	ATOM	2025	O	VAL	B	316	15.397	6.579	34.318	1.00	25.55
	ATOM	2026	N	SER	B	317	16.601	8.243	35.242	1.00	24.40
50	ATOM	2027	CA	SER	B	317	15.799	8.268	36.460	1.00	27.63
	ATOM	2028	CB	SER	B	317	16.358	9.294	37.451	1.00	31.68
	ATOM	2029	OG	SER	B	317	17.492	8.771	38.112	1.00	39.97
	ATOM	2030	C	SER	B	317	14.346	8.600	36.154	1.00	26.73
	ATOM	2031	O	SER	B	317	13.434	7.932	36.648	1.00	25.65
55	ATOM	2032	N	ALA	B	318	14.135	9.634	35.342	1.00	24.19
	ATOM	2033	CA	ALA	B	318	12.786	10.049	34.969	1.00	24.17
	ATOM	2034	CB	ALA	B	318	12.850	11.250	34.022	1.00	21.44
	ATOM	2035	C	ALA	B	318	12.038	8.890	34.306	1.00	21.63
	ATOM	2036	O	ALA	B	318	10.902	8.598	34.648	1.00	20.25
60	ATOM	2037	N	LEU	B	319	12.695	8.225	33.364	1.00	23.37
	ATOM	2038	CA	LEU	B	319	12.098	7.102	32.652	1.00	25.42

5	ATOM	2039	CB	LEU	B	319	13.050	6.635	31.548	1.00	22.03
	ATOM	2040	CG	LEU	B	319	13.264	7.622	30.394	1.00	20.71
	ATOM	2041	CD1	LEU	B	319	14.146	6.995	29.331	1.00	23.60
	ATOM	2042	CD2	LEU	B	319	11.918	8.020	29.803	1.00	23.82
	ATOM	2043	C	LEU	B	319	11.729	5.926	33.564	1.00	27.26
10	ATOM	2044	O	LEU	B	319	10.615	5.396	33.488	1.00	28.91
	ATOM	2045	N	LEU	B	320	12.656	5.516	34.426	1.00	26.58
	ATOM	2046	CA	LEU	B	320	12.399	4.405	35.334	1.00	26.73
	ATOM	2047	CB	LEU	B	320	13.657	4.075	36.145	1.00	26.87
	ATOM	2048	CG	LEU	B	320	14.846	3.460	35.398	1.00	26.15
15	ATOM	2049	CD1	LEU	B	320	16.053	3.375	36.330	1.00	28.04
	ATOM	2050	CD2	LEU	B	320	14.484	2.076	34.895	1.00	26.96
	ATOM	2051	C	LEU	B	320	11.249	4.722	36.290	1.00	29.19
	ATOM	2052	O	LEU	B	320	10.449	3.849	36.631	1.00	26.66
	ATOM	2053	N	ASP	B	321	11.160	5.976	36.719	1.00	29.72
20	ATOM	2054	CA	ASP	B	321	10.112	6.371	37.647	1.00	31.36
	ATOM	2055	CB	ASP	B	321	10.494	7.683	38.336	1.00	36.60
	ATOM	2056	CG	ASP	B	321	11.407	7.461	39.535	1.00	46.11
	ATOM	2057	OD1	ASP	B	321	10.897	7.058	40.605	1.00	46.64
	ATOM	2058	OD2	ASP	B	321	12.635	7.676	39.402	1.00	45.98
25	ATOM	2059	C	ASP	B	321	8.742	6.494	36.989	1.00	28.29
	ATOM	2060	O	ASP	B	321	7.715	6.432	37.661	1.00	27.19
	ATOM	2061	N	ALA	B	322	8.726	6.650	35.672	1.00	28.34
	ATOM	2062	CA	ALA	B	322	7.469	6.779	34.950	1.00	25.55
	ATOM	2063	CB	ALA	B	322	7.668	7.668	33.728	1.00	24.11
30	ATOM	2064	C	ALA	B	322	6.911	5.420	34.523	1.00	22.80
	ATOM	2065	O	ALA	B	322	5.810	5.338	33.979	1.00	24.54
	ATOM	2066	N	GLU	B	323	7.662	4.355	34.781	1.00	20.16
	ATOM	2067	CA	GLU	B	323	7.229	3.021	34.386	1.00	21.44
	ATOM	2068	CB	GLU	B	323	8.196	1.982	34.938	1.00	23.72
35	ATOM	2069	CG	GLU	B	323	9.393	1.746	34.024	1.00	23.58
	ATOM	2070	CD	GLU	B	323	8.988	1.134	32.685	1.00	25.23
	ATOM	2071	OE1	GLU	B	323	8.852	1.881	31.692	1.00	21.74
	ATOM	2072	OE2	GLU	B	323	8.809	-0.095	32.624	1.00	25.49
	ATOM	2073	C	GLU	B	323	5.796	2.696	34.810	1.00	22.35
40	ATOM	2074	O	GLU	B	323	5.409	2.926	35.951	1.00	22.34
	ATOM	2075	N	PRO	B	324	4.986	2.165	33.880	1.00	19.10
	ATOM	2076	CD	PRO	B	324	5.286	1.806	32.483	1.00	19.11
	ATOM	2077	CA	PRO	B	324	3.607	1.839	34.242	1.00	22.04
	ATOM	2078	CB	PRO	B	324	2.919	1.658	32.893	1.00	21.96
45	ATOM	2079	CG	PRO	B	324	4.015	1.137	32.015	1.00	24.13
	ATOM	2080	C	PRO	B	324	3.619	0.556	35.060	1.00	23.44
	ATOM	2081	O	PRO	B	324	4.590	-0.200	35.028	1.00	22.20
	ATOM	2082	N	PRO	B	325	2.540	0.287	35.801	1.00	24.88
	ATOM	2083	CD	PRO	B	325	1.299	1.068	35.945	1.00	26.67
50	ATOM	2084	CA	PRO	B	325	2.520	-0.940	36.603	1.00	25.10
	ATOM	2085	CB	PRO	B	325	1.394	-0.691	37.595	1.00	27.09
	ATOM	2086	CG	PRO	B	325	0.448	0.205	36.854	1.00	26.87
	ATOM	2087	C	PRO	B	325	2.270	-2.192	35.776	1.00	25.77
	ATOM	2088	O	PRO	B	325	1.853	-2.118	34.617	1.00	21.69
55	ATOM	2089	N	ILE	B	326	2.538	-3.344	36.379	1.00	24.05
	ATOM	2090	CA	ILE	B	326	2.301	-4.620	35.722	1.00	22.51
	ATOM	2091	CB	ILE	B	326	3.303	-5.688	36.185	1.00	25.81
	ATOM	2092	CG2	ILE	B	326	3.011	-7.018	35.481	1.00	23.78
	ATOM	2093	CG1	ILE	B	326	4.729	-5.209	35.900	1.00	25.75
60	ATOM	2094	CD1	ILE	B	326	5.241	-5.585	34.533	1.00	27.78
	ATOM	2095	C	ILE	B	326	0.893	-5.020	36.149	1.00	23.63

5	ATOM	2096	O	ILE	B	326	0.632	-5.231	37.332	1.00	24.81
	ATOM	2097	N	LEU	B	327	-0.018	-5.104	35.188	1.00	19.44
	ATOM	2098	CA	LEU	B	327	-1.399	-5.437	35.493	1.00	17.03
	ATOM	2099	CB	LEU	B	327	-2.336	-4.747	34.493	1.00	18.39
	ATOM	2100	CG	LEU	B	327	-2.201	-3.216	34.373	1.00	20.69
10	ATOM	2101	CD1	LEU	B	327	-3.245	-2.679	33.406	1.00	14.87
	ATOM	2102	CD2	LEU	B	327	-2.384	-2.570	35.742	1.00	14.39
	ATOM	2103	C	LEU	B	327	-1.662	-6.928	35.499	1.00	19.87
	ATOM	2104	O	LEU	B	327	-0.854	-7.722	35.014	1.00	20.90
	ATOM	2105	N	TYR	B	328	-2.803	-7.300	36.066	1.00	20.92
15	ATOM	2106	CA	TYR	B	328	-3.202	-8.692	36.135	1.00	21.79
	ATOM	2107	CB	TYR	B	328	-3.658	-9.050	37.550	1.00	22.91
	ATOM	2108	CG	TYR	B	328	-2.515	-9.376	38.468	1.00	24.60
	ATOM	2109	CD1	TYR	B	328	-2.118	-10.696	38.677	1.00	25.93
	ATOM	2110	CE1	TYR	B	328	-1.034	-11.000	39.498	1.00	28.10
20	ATOM	2111	CD2	TYR	B	328	-1.802	-8.362	39.103	1.00	29.46
	ATOM	2112	CE2	TYR	B	328	-0.716	-8.654	39.926	1.00	35.30
	ATOM	2113	CZ	TYR	B	328	-0.338	-9.973	40.117	1.00	32.59
	ATOM	2114	OH	TYR	B	328	0.739	-10.257	40.923	1.00	37.24
	ATOM	2115	C	TYR	B	328	-4.336	-8.944	35.168	1.00	22.25
25	ATOM	2116	O	TYR	B	328	-5.115	-8.039	34.849	1.00	19.77
	ATOM	2117	N	SER	B	329	-4.420	-10.180	34.698	1.00	25.81
	ATOM	2118	CA	SER	B	329	-5.480	-10.571	33.787	1.00	29.39
	ATOM	2119	CB	SER	B	329	-5.002	-11.710	32.887	1.00	27.65
	ATOM	2120	OG	SER	B	329	-6.091	-12.329	32.233	1.00	28.98
30	ATOM	2121	C	SER	B	329	-6.625	-11.042	34.673	1.00	33.17
	ATOM	2122	O	SER	B	329	-6.453	-11.157	35.888	1.00	32.52
	ATOM	2123	N	GLU	B	330	-7.792	-11.289	34.084	1.00	38.75
	ATOM	2124	CA	GLU	B	330	-8.930	-11.776	34.859	1.00	44.91
	ATOM	2125	CB	GLU	B	330	-10.134	-11.999	33.951	1.00	45.63
35	ATOM	2126	C	GLU	B	330	-8.493	-13.093	35.491	1.00	48.62
	ATOM	2127	O	GLU	B	330	-7.739	-13.851	34.882	1.00	52.37
	ATOM	2128	N	TYR	B	331	-8.952	-13.366	36.707	1.00	51.75
	ATOM	2129	CA	TYR	B	331	-8.575	-14.596	37.396	1.00	55.25
	ATOM	2130	CB	TYR	B	331	-8.538	-14.365	38.911	1.00	53.04
40	ATOM	2131	CG	TYR	B	331	-9.769	-13.668	39.440	1.00	50.70
	ATOM	2132	CD1	TYR	B	331	-10.880	-14.400	39.856	1.00	47.09
	ATOM	2133	CE1	TYR	B	331	-12.035	-13.762	40.292	1.00	46.43
	ATOM	2134	CD2	TYR	B	331	-9.842	-12.273	39.478	1.00	47.52
	ATOM	2135	CE2	TYR	B	331	-10.993	-11.625	39.913	1.00	43.98
45	ATOM	2136	CZ	TYR	B	331	-12.086	-12.376	40.314	1.00	44.33
	ATOM	2137	OH	TYR	B	331	-13.239	-11.747	40.715	1.00	45.31
	ATOM	2138	C	TYR	B	331	-9.528	-15.743	37.075	1.00	60.11
	ATOM	2139	O	TYR	B	331	-10.748	-15.569	37.066	1.00	63.13
	ATOM	2140	N	ASP	B	332	-8.952	-16.913	36.809	1.00	61.60
50	ATOM	2141	CA	ASP	B	332	-9.704	-18.124	36.490	1.00	63.58
	ATOM	2142	CB	ASP	B	332	-10.637	-17.895	35.298	1.00	65.11
	ATOM	2143	CG	ASP	B	332	-11.723	-18.953	35.200	1.00	65.32
	ATOM	2144	OD1	ASP	B	332	-11.420	-20.136	35.463	1.00	63.69
	ATOM	2145	OD2	ASP	B	332	-12.876	-18.602	34.866	1.00	63.61
55	ATOM	2146	C	ASP	B	332	-8.707	-19.227	36.153	1.00	62.86
	ATOM	2147	O	ASP	B	332	-7.853	-19.056	35.287	1.00	62.26
	ATOM	2148	N	PRO	B	333	-8.811	-20.379	36.833	1.00	63.96
	ATOM	2149	CD	PRO	B	333	-9.808	-20.690	37.875	1.00	64.24
	ATOM	2150	CA	PRO	B	333	-7.901	-21.503	36.596	1.00	64.24
60	ATOM	2151	CB	PRO	B	333	-8.015	-22.325	37.874	1.00	64.70
	ATOM	2152	CG	PRO	B	333	-9.410	-22.071	38.347	1.00	65.00

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5	ATOM	2153	C	PRO	B	333	-8.180	-22.340	35.351	1.00	63.90
	ATOM	2154	O	PRO	B	333	-7.384	-23.214	35.007	1.00	63.70
	ATOM	2155	N	THR	B	334	-9.303	-22.084	34.683	1.00	63.83
10	ATOM	2156	CA	THR	B	334	-9.649	-22.832	33.475	1.00	63.77
	ATOM	2157	CB	THR	B	334	-11.065	-22.477	32.975	1.00	64.63
	ATOM	2158	OG1	THR	B	334	-11.132	-21.078	32.675	1.00	65.95
	ATOM	2159	CG2	THR	B	334	-12.102	-22.817	34.036	1.00	65.09
	ATOM	2160	C	THR	B	334	-8.634	-22.499	32.388	1.00	62.62
15	ATOM	2161	O	THR	B	334	-8.931	-21.774	31.437	1.00	60.15
	ATOM	2162	N	ARG	B	335	-7.432	-23.043	32.553	1.00	63.14
	ATOM	2163	CA	ARG	B	335	-6.324	-22.820	31.633	1.00	60.70
	ATOM	2164	CB	ARG	B	335	-5.130	-23.667	32.050	1.00	58.73
	ATOM	2165	C	ARG	B	335	-6.667	-23.086	30.174	1.00	59.71
20	ATOM	2166	O	ARG	B	335	-6.302	-22.298	29.298	1.00	62.33
	ATOM	2167	N	PRO	B	336	-7.377	-24.194	29.884	1.00	55.25
	ATOM	2168	CD	PRO	B	336	-7.938	-25.227	30.769	1.00	53.53
	ATOM	2169	CA	PRO	B	336	-7.698	-24.437	28.471	1.00	50.10
	ATOM	2170	CB	PRO	B	336	-8.399	-25.799	28.476	1.00	49.70
25	ATOM	2171	CG	PRO	B	336	-8.164	-26.372	29.844	1.00	50.71
	ATOM	2172	C	PRO	B	336	-8.602	-23.324	27.954	1.00	44.54
	ATOM	2173	O	PRO	B	336	-9.809	-23.342	28.179	1.00	44.14
	ATOM	2174	N	PHE	B	337	-8.007	-22.350	27.274	1.00	39.18
	ATOM	2175	CA	PHE	B	337	-8.764	-21.223	26.742	1.00	38.25
30	ATOM	2176	CB	PHE	B	337	-7.850	-20.003	26.567	1.00	36.98
	ATOM	2177	CG	PHE	B	337	-7.229	-19.517	27.846	1.00	36.81
	ATOM	2178	CD1	PHE	B	337	-5.846	-19.511	28.002	1.00	38.89
	ATOM	2179	CD2	PHE	B	337	-8.023	-19.062	28.893	1.00	35.97
	ATOM	2180	CE1	PHE	B	337	-5.262	-19.059	29.185	1.00	36.85
35	ATOM	2181	CE2	PHE	B	337	-7.449	-18.608	30.079	1.00	37.15
	ATOM	2182	CZ	PHE	B	337	-6.064	-18.607	30.224	1.00	38.40
	ATOM	2183	C	PHE	B	337	-9.420	-21.535	25.402	1.00	36.81
	ATOM	2184	O	PHE	B	337	-8.962	-22.399	24.658	1.00	36.26
	ATOM	2185	N	SER	B	338	-10.504	-20.828	25.107	1.00	35.85
40	ATOM	2186	CA	SER	B	338	-11.198	-20.981	23.836	1.00	34.76
	ATOM	2187	CB	SER	B	338	-12.713	-20.948	24.035	1.00	34.85
	ATOM	2188	OG	SER	B	338	-13.164	-19.621	24.235	1.00	33.53
	ATOM	2189	C	SER	B	338	-10.761	-19.761	23.037	1.00	34.99
	ATOM	2190	O	SER	B	338	-10.143	-18.855	23.591	1.00	34.32
45	ATOM	2191	N	GLU	B	339	-11.075	-19.722	21.750	1.00	33.01
	ATOM	2192	CA	GLU	B	339	-10.682	-18.579	20.950	1.00	33.94
	ATOM	2193	CB	GLU	B	339	-11.146	-18.737	19.501	1.00	33.79
	ATOM	2194	CG	GLU	B	339	-10.758	-17.553	18.623	1.00	39.11
	ATOM	2195	CD	GLU	B	339	-10.865	-17.852	17.137	1.00	43.17
50	ATOM	2196	OE1	GLU	B	339	-11.990	-17.785	16.600	1.00	45.28
	ATOM	2197	OE2	GLU	B	339	-9.824	-18.152	16.510	1.00	39.19
	ATOM	2198	C	GLU	B	339	-11.265	-17.295	21.531	1.00	34.28
	ATOM	2199	O	GLU	B	339	-10.575	-16.283	21.631	1.00	33.65
	ATOM	2200	N	ALA	B	340	-12.535	-17.339	21.920	1.00	31.12
55	ATOM	2201	CA	ALA	B	340	-13.194	-16.164	22.469	1.00	29.10
	ATOM	2202	CB	ALA	B	340	-14.696	-16.412	22.573	1.00	33.84
	ATOM	2203	C	ALA	B	340	-12.639	-15.731	23.826	1.00	28.98
	ATOM	2204	O	ALA	B	340	-12.431	-14.541	24.060	1.00	30.48
	ATOM	2205	N	SER	B	341	-12.407	-16.691	24.719	1.00	26.66
60	ATOM	2206	CA	SER	B	341	-11.882	-16.386	26.044	1.00	24.26
	ATOM	2207	CB	SER	B	341	-11.867	-17.643	26.923	1.00	27.04
	ATOM	2208	OG	SER	B	341	-10.851	-18.541	26.515	1.00	33.84
	ATOM	2209	C	SER	B	341	-10.479	-15.793	25.960	1.00	23.97

5	ATOM	2210	O	SER	B	341	-10.171	-14.824	26.651	1.00	21.56
	ATOM	2211	N	MET	B	342	-9.631	-16.368	25.114	1.00	26.83
	ATOM	2212	CA	MET	B	342	-8.271	-15.865	24.954	1.00	27.24
	ATOM	2213	CB	MET	B	342	-7.477	-16.758	24.001	1.00	30.45
	ATOM	2214	CG	MET	B	342	-6.038	-16.300	23.802	1.00	35.35
10	ATOM	2215	SD	MET	B	342	-4.866	-17.667	23.777	1.00	44.57
	ATOM	2216	CE	MET	B	342	-4.034	-17.341	22.244	1.00	41.37
	ATOM	2217	C	MET	B	342	-8.322	-14.448	24.385	1.00	25.31
	ATOM	2218	O	MET	B	342	-7.653	-13.541	24.874	1.00	26.67
	ATOM	2219	N	MET	B	343	-9.114	-14.278	23.345	1.00	25.75
15	ATOM	2220	CA	MET	B	343	-9.262	-12.979	22.712	1.00	25.47
	ATOM	2221	CB	MET	B	343	-10.210	-13.088	21.528	1.00	23.51
	ATOM	2222	CG	MET	B	343	-9.540	-13.618	20.273	1.00	28.86
	ATOM	2223	SD	MET	B	343	-8.325	-12.456	19.609	1.00	29.25
	ATOM	2224	CE	MET	B	343	-9.344	-11.015	19.371	1.00	28.74
20	ATOM	2225	C	MET	B	343	-9.798	-11.966	23.712	1.00	25.37
	ATOM	2226	O	MET	B	343	-9.360	-10.810	23.728	1.00	24.98
	ATOM	2227	N	GLY	B	344	-10.739	-12.403	24.536	1.00	23.91
	ATOM	2228	CA	GLY	B	344	-11.320	-11.526	25.536	1.00	22.43
	ATOM	2229	C	GLY	B	344	-10.313	-11.103	26.592	1.00	22.06
25	ATOM	2230	O	GLY	B	344	-10.262	-9.934	26.982	1.00	20.87
	ATOM	2231	N	LEU	B	345	-9.511	-12.048	27.063	1.00	19.36
	ATOM	2232	CA	LEU	B	345	-8.520	-11.748	28.083	1.00	25.74
	ATOM	2233	CB	LEU	B	345	-7.886	-13.040	28.600	1.00	26.78
	ATOM	2234	CG	LEU	B	345	-8.794	-14.010	29.362	1.00	30.04
30	ATOM	2235	CD1	LEU	B	345	-8.099	-15.357	29.488	1.00	28.39
	ATOM	2236	CD2	LEU	B	345	-9.122	-13.443	30.736	1.00	29.93
	ATOM	2237	C	LEU	B	345	-7.425	-10.822	27.550	1.00	23.24
	ATOM	2238	O	LEU	B	345	-7.037	-9.865	28.212	1.00	23.43
	ATOM	2239	N	LEU	B	346	-6.937	-11.108	26.350	1.00	21.92
35	ATOM	2240	CA	LEU	B	346	-5.874	-10.303	25.763	1.00	22.71
	ATOM	2241	CB	LEU	B	346	-5.343	-10.962	24.486	1.00	23.17
	ATOM	2242	CG	LEU	B	346	-4.684	-12.331	24.668	1.00	20.66
	ATOM	2243	CD1	LEU	B	346	-4.303	-12.916	23.309	1.00	18.75
	ATOM	2244	CD2	LEU	B	346	-3.464	-12.188	25.553	1.00	20.84
40	ATOM	2245	C	LEU	B	346	-6.304	-8.873	25.458	1.00	22.99
	ATOM	2246	O	LEU	B	346	-5.540	-7.935	25.695	1.00	22.07
	ATOM	2247	N	THR	B	347	-7.516	-8.699	24.937	1.00	20.53
	ATOM	2248	CA	THR	B	347	-7.987	-7.357	24.608	1.00	21.89
	ATOM	2249	CB	THR	B	347	-9.152	-7.388	23.601	1.00	21.65
45	ATOM	2250	OG1	THR	B	347	-10.218	-8.190	24.123	1.00	19.65
	ATOM	2251	CG2	THR	B	347	-8.676	-7.955	22.262	1.00	22.01
	ATOM	2252	C	THR	B	347	-8.426	-6.590	25.853	1.00	23.60
	ATOM	2253	O	THR	B	347	-8.358	-5.357	25.883	1.00	20.31
	ATOM	2254	N	ASN	B	348	-8.884	-7.314	26.874	1.00	22.27
50	ATOM	2255	CA	ASN	B	348	-9.293	-6.667	28.114	1.00	23.99
	ATOM	2256	CB	ASN	B	348	-10.008	-7.642	29.056	1.00	22.32
	ATOM	2257	CG	ASN	B	348	-10.342	-7.022	30.398	1.00	28.26
	ATOM	2258	OD1	ASN	B	348	-9.478	-6.746	31.216	1.00	27.14
	ATOM	2259	ND2	ASN	B	348	-11.647	-6.764	30.625	1.00	27.02
55	ATOM	2260	C	ASN	B	348	-8.035	-6.120	28.798	1.00	19.48
	ATOM	2261	O	ASN	B	348	-8.014	-4.991	29.271	1.00	18.26
	ATOM	2262	N	LEU	B	349	-6.984	-6.931	28.832	1.00	19.07
	ATOM	2263	CA	LEU	B	349	-5.724	-6.516	29.446	1.00	20.37
	ATOM	2264	CB	LEU	B	349	-4.716	-7.674	29.434	1.00	18.21
60	ATOM	2265	CG	LEU	B	349	-3.297	-7.316	29.889	1.00	18.24
	ATOM	2266	CD1	LEU	B	349	-3.323	-6.904	31.356	1.00	12.44

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5	ATOM	2324	CE1	HIS	B	356	-2.802	1.860	36.145	1.00	18.84
	ATOM	2325	NE2	HIS	B	356	-3.598	1.088	35.426	1.00	17.92
	ATOM	2326	C	HIS	B	356	-0.479	3.861	31.184	1.00	19.67
	ATOM	2327	O	HIS	B	356	0.424	4.614	31.547	1.00	19.61
	ATOM	2328	N	MET	B	357	-0.566	3.413	29.931	1.00	14.92
10	ATOM	2329	CA	MET	B	357	0.428	3.830	28.939	1.00	15.13
	ATOM	2330	CB	MET	B	357	0.239	3.099	27.604	1.00	13.94
	ATOM	2331	CG	MET	B	357	1.149	3.631	26.476	1.00	14.71
	ATOM	2332	SD	MET	B	357	0.747	3.014	24.826	1.00	17.75
	ATOM	2333	CE	MET	B	357	0.746	1.222	25.122	1.00	15.21
15	ATOM	2334	C	MET	B	357	0.316	5.334	28.699	1.00	14.94
	ATOM	2335	O	MET	B	357	1.319	6.031	28.560	1.00	17.02
	ATOM	2336	N	ILE	B	358	-0.909	5.839	28.659	1.00	18.01
	ATOM	2337	CA	ILE	B	358	-1.122	7.263	28.423	1.00	19.77
	ATOM	2338	CB	ILE	B	358	-2.634	7.577	28.287	1.00	23.11
20	ATOM	2339	CG2	ILE	B	358	-2.879	9.080	28.450	1.00	25.00
	ATOM	2340	CG1	ILE	B	358	-3.137	7.105	26.913	1.00	24.19
	ATOM	2341	CD1	ILE	B	358	-4.600	6.653	26.890	1.00	20.17
	ATOM	2342	C	ILE	B	358	-0.501	8.100	29.550	1.00	22.93
	ATOM	2343	O	ILE	B	358	0.080	9.153	29.299	1.00	23.33
25	ATOM	2344	N	ASN	B	359	-0.619	7.631	30.790	1.00	22.34
	ATOM	2345	CA	ASN	B	359	-0.029	8.341	31.924	1.00	23.24
	ATOM	2346	CB	ASN	B	359	-0.480	7.726	33.224	1.00	25.10
	ATOM	2347	CG	ASN	B	359	-1.831	8.171	33.649	1.00	32.65
	ATOM	2348	OD1	ASN	B	359	-2.421	9.069	33.042	1.00	32.98
30	ATOM	2349	ND2	ASN	B	359	-2.364	7.549	34.691	1.00	33.87
	ATOM	2350	C	ASN	B	359	1.473	8.306	31.837	1.00	24.77
	ATOM	2351	O	ASN	B	359	2.152	9.285	32.149	1.00	24.19
	ATOM	2352	N	TRP	B	360	1.995	7.149	31.438	1.00	20.82
	ATOM	2353	CA	TRP	B	360	3.439	6.965	31.310	1.00	19.29
35	ATOM	2354	CB	TRP	B	360	3.754	5.524	30.878	1.00	18.59
	ATOM	2355	CG	TRP	B	360	5.085	5.363	30.176	1.00	18.21
	ATOM	2356	CD2	TRP	B	360	5.310	5.308	28.756	1.00	14.38
	ATOM	2357	CE2	TRP	B	360	6.698	5.129	28.561	1.00	13.42
	ATOM	2358	CE3	TRP	B	360	4.475	5.392	27.633	1.00	15.52
40	ATOM	2359	CD1	TRP	B	360	6.306	5.221	30.762	1.00	13.34
	ATOM	2360	NE1	TRP	B	360	7.283	5.078	29.800	1.00	16.05
	ATOM	2361	CZ2	TRP	B	360	7.272	5.032	27.288	1.00	16.84
	ATOM	2362	CZ3	TRP	B	360	5.045	5.296	26.363	1.00	15.11
	ATOM	2363	CH2	TRP	B	360	6.431	5.115	26.202	1.00	16.12
45	ATOM	2364	C	TRP	B	360	3.979	7.939	30.273	1.00	20.13
	ATOM	2365	O	TRP	B	360	4.991	8.606	30.497	1.00	17.26
	ATOM	2366	N	ALA	B	361	3.295	8.012	29.135	1.00	19.34
	ATOM	2367	CA	ALA	B	361	3.708	8.900	28.051	1.00	22.01
	ATOM	2368	CB	ALA	B	361	2.682	8.855	26.921	1.00	19.53
50	ATOM	2369	C	ALA	B	361	3.883	10.336	28.552	1.00	22.39
	ATOM	2370	O	ALA	B	361	4.858	11.005	28.210	1.00	19.57
	ATOM	2371	N	LYS	B	362	2.932	10.794	29.361	1.00	21.96
	ATOM	2372	CA	LYS	B	362	2.966	12.139	29.923	1.00	26.45
	ATOM	2373	CB	LYS	B	362	1.741	12.363	30.811	1.00	29.79
55	ATOM	2374	CG	LYS	B	362	0.426	12.417	30.064	1.00	33.57
	ATOM	2375	CD	LYS	B	362	-0.563	13.304	30.805	1.00	36.83
	ATOM	2376	CE	LYS	B	362	-1.620	12.490	31.512	1.00	36.89
	ATOM	2377	NZ	LYS	B	362	-2.873	13.276	31.664	1.00	39.07
	ATOM	2378	C	LYS	B	362	4.223	12.379	30.757	1.00	27.77
60	ATOM	2379	O	LYS	B	362	4.661	13.517	30.922	1.00	26.93
	ATOM	2380	N	ARG	B	363	4.805	11.302	31.278	1.00	26.61

							5.996	11.414	32.109	1.00	27.74
5	ATOM	2381	CA	ARG	B	363	5.887	10.457	33.298	1.00	28.93
	ATOM	2382	CB	ARG	B	363	4.650	10.704	34.158	1.00	36.07
	ATOM	2383	CG	ARG	B	363	4.569	9.745	35.344	1.00	42.83
	ATOM	2384	CD	ARG	B	363	4.477	8.344	34.928	1.00	49.79
	ATOM	2385	NE	ARG	B	363	3.395	7.582	35.080	1.00	51.48
10	ATOM	2386	CZ	ARG	B	363	2.300	8.081	35.648	1.00	52.17
	ATOM	2387	NH1	ARG	B	363	3.405	6.316	34.668	1.00	40.24
	ATOM	2388	NH2	ARG	B	363	7.308	11.190	31.367	1.00	25.80
	ATOM	2389	C	ARG	B	363	8.374	11.183	31.975	1.00	29.36
	ATOM	2390	O	ARG	B	363	7.231	11.009	30.053	1.00	24.28
15	ATOM	2391	N	VAL	B	364	8.431	10.823	29.248	1.00	21.87
	ATOM	2392	CA	VAL	B	364	8.116	10.048	27.947	1.00	21.84
	ATOM	2393	CB	VAL	B	364	9.267	10.184	26.968	1.00	15.85
	ATOM	2394	CG1	VAL	B	364	7.860	8.560	28.268	1.00	16.24
	ATOM	2395	CG2	VAL	B	364	8.925	12.241	28.923	1.00	28.14
20	ATOM	2396	C	VAL	B	364	8.219	13.023	28.285	1.00	24.24
	ATOM	2397	O	VAL	B	364	10.141	12.591	29.375	1.00	28.57
	ATOM	2398	N	PRO	B	365	11.061	11.726	30.137	1.00	30.58
	ATOM	2399	CD	PRO	B	365	10.719	13.919	29.138	1.00	32.16
	ATOM	2400	CA	PRO	B	365	12.189	13.739	29.507	1.00	32.70
25	ATOM	2401	CB	PRO	B	365	12.170	12.671	30.545	1.00	33.35
	ATOM	2402	CG	PRO	B	365	10.546	14.464	27.726	1.00	32.22
	ATOM	2403	C	PRO	B	365	11.056	13.897	26.766	1.00	37.04
	ATOM	2404	O	PRO	B	365	9.821	15.570	27.609	1.00	34.09
	ATOM	2405	N	GLY	B	366	9.612	16.182	26.310	1.00	32.54
30	ATOM	2406	CA	GLY	B	366	8.241	15.969	25.700	1.00	33.46
	ATOM	2407	C	GLY	B	366	7.791	16.779	24.886	1.00	33.73
	ATOM	2408	O	GLY	B	366	7.564	14.895	26.096	1.00	31.08
	ATOM	2409	N	PHE	B	367	6.250	14.593	25.542	1.00	28.60
	ATOM	2410	CA	PHE	B	367	5.745	13.244	26.058	1.00	25.96
35	ATOM	2411	CB	PHE	B	367	4.629	12.671	25.239	1.00	22.75
	ATOM	2412	CG	PHE	B	367	3.313	12.771	25.669	1.00	22.62
	ATOM	2413	CD1	PHE	B	367	4.897	12.025	24.033	1.00	22.29
	ATOM	2414	CD2	PHE	B	367	2.272	12.233	24.914	1.00	25.63
	ATOM	2415	CE1	PHE	B	367	3.867	11.486	23.272	1.00	20.82
40	ATOM	2416	CE2	PHE	B	367	2.553	11.588	23.711	1.00	25.50
	ATOM	2417	CZ	PHE	B	367	5.178	15.646	25.781	1.00	26.79
	ATOM	2418	C	PHE	B	367	4.458	16.001	24.854	1.00	23.37
	ATOM	2419	O	PHE	B	367	5.049	16.143	27.009	1.00	31.26
	ATOM	2420	N	VAL	B	368	4.020	17.151	27.277	1.00	35.71
45	ATOM	2421	CA	VAL	B	368	3.817	17.412	28.795	1.00	35.98
	ATOM	2422	CB	VAL	B	368	2.944	16.320	29.392	1.00	37.64
	ATOM	2423	CG1	VAL	B	368	5.157	17.495	29.508	1.00	35.81
	ATOM	2424	CG2	VAL	B	368	4.328	18.482	26.598	1.00	35.87
	ATOM	2425	C	VAL	B	368	3.450	19.330	26.457	1.00	37.71
50	ATOM	2426	O	VAL	B	368	5.572	18.665	26.175	1.00	35.49
	ATOM	2427	N	ASP	B	369	5.950	19.904	25.503	1.00	36.54
	ATOM	2428	CA	ASP	B	369	7.466	19.963	25.309	1.00	39.79
	ATOM	2429	CB	ASP	B	369	8.213	20.169	26.615	1.00	44.33
	ATOM	2430	CG	ASP	B	369	9.409	19.807	26.684	1.00	48.45
55	ATOM	2431	OD1	ASP	B	369	7.604	20.693	27.572	1.00	43.27
	ATOM	2432	OD2	ASP	B	369	5.248	19.997	24.149	1.00	34.49
	ATOM	2433	C	ASP	B	369	5.131	21.074	23.571	1.00	34.51
	ATOM	2434	O	ASP	B	369	4.776	18.859	23.653	1.00	30.97
	ATOM	2435	N	LEU	B	370	4.086	18.809	22.370	1.00	29.80
60	ATOM	2436	CA	LEU	B	370	4.145	17.389	21.799	1.00	27.27
	ATOM	2437	CB	LEU	B	370					

5	ATOM	2438	CG	LEU	B	370	5.522	16.733	21.688	1.00	28.07
	ATOM	2439	CD1	LEU	B	370	5.353	15.242	21.400	1.00	30.38
	ATOM	2440	CD2	LEU	B	370	6.316	17.396	20.574	1.00	22.82
	ATOM	2441	C	LEU	B	370	2.628	19.218	22.521	1.00	28.04
	ATOM	2442	O	LEU	B	370	2.066	19.151	23.611	1.00	29.71
10	ATOM	2443	N	THR	B	371	2.011	19.645	21.425	1.00	28.70
	ATOM	2444	CA	THR	B	371	0.602	20.014	21.474	1.00	30.31
	ATOM	2445	CB	THR	B	371	0.150	20.690	20.163	1.00	31.96
	ATOM	2446	OG1	THR	B	371	0.284	19.763	19.080	1.00	29.49
	ATOM	2447	CG2	THR	B	371	0.991	21.930	19.878	1.00	29.98
15	ATOM	2448	C	THR	B	371	-0.208	18.726	21.666	1.00	30.59
	ATOM	2449	O	THR	B	371	0.300	17.624	21.431	1.00	27.10
	ATOM	2450	N	LEU	B	372	-1.461	18.863	22.087	1.00	27.65
	ATOM	2451	CA	LEU	B	372	-2.323	17.702	22.303	1.00	30.86
	ATOM	2452	CB	LEU	B	372	-3.722	18.147	22.737	1.00	30.11
20	ATOM	2453	CG	LEU	B	372	-4.715	17.006	22.960	1.00	32.80
	ATOM	2454	CD1	LEU	B	372	-4.231	16.147	24.126	1.00	34.10
	ATOM	2455	CD2	LEU	B	372	-6.105	17.562	23.246	1.00	31.16
	ATOM	2456	C	LEU	B	372	-2.437	16.863	21.034	1.00	31.77
	ATOM	2457	O	LEU	B	372	-2.417	15.629	21.078	1.00	27.06
25	ATOM	2458	N	HIS	B	373	-2.564	17.548	19.905	1.00	31.30
	ATOM	2459	CA	HIS	B	373	-2.685	16.888	18.614	1.00	31.35
	ATOM	2460	CB	HIS	B	373	-2.844	17.935	17.503	1.00	34.30
	ATOM	2461	CG	HIS	B	373	-2.503	17.430	16.132	1.00	41.27
	ATOM	2462	CD2	HIS	B	373	-3.293	17.105	15.079	1.00	42.50
30	ATOM	2463	ND1	HIS	B	373	-1.205	17.220	15.715	1.00	43.69
	ATOM	2464	CE1	HIS	B	373	-1.210	16.787	14.465	1.00	48.87
	ATOM	2465	NE2	HIS	B	373	-2.465	16.708	14.056	1.00	43.72
	ATOM	2466	C	HIS	B	373	-1.468	16.012	18.337	1.00	28.29
	ATOM	2467	O	HIS	B	373	-1.610	14.878	17.897	1.00	30.21
35	ATOM	2468	N	ASP	B	374	-0.275	16.541	18.589	1.00	28.85
	ATOM	2469	CA	ASP	B	374	0.950	15.783	18.350	1.00	28.28
	ATOM	2470	CB	ASP	B	374	2.178	16.678	18.535	1.00	31.33
	ATOM	2471	CG	ASP	B	374	2.433	17.577	17.333	1.00	39.07
	ATOM	2472	OD1	ASP	B	374	3.195	18.557	17.478	1.00	40.60
40	ATOM	2473	OD2	ASP	B	374	1.874	17.305	16.246	1.00	38.64
	ATOM	2474	C	ASP	B	374	1.029	14.592	19.303	1.00	29.05
	ATOM	2475	O	ASP	B	374	1.432	13.494	18.908	1.00	24.26
	ATOM	2476	N	GLN	B	375	0.642	14.814	20.556	1.00	24.52
	ATOM	2477	CA	GLN	B	375	0.667	13.749	21.547	1.00	27.37
45	ATOM	2478	CB	GLN	B	375	0.213	14.270	22.901	1.00	26.66
	ATOM	2479	CG	GLN	B	375	1.164	15.236	23.563	1.00	29.74
	ATOM	2480	CD	GLN	B	375	0.623	15.691	24.890	1.00	33.13
	ATOM	2481	OE1	GLN	B	375	-0.044	14.953	25.602	1.00	32.82
	ATOM	2482	NE2	GLN	B	375	0.895	16.953	25.236	1.00	33.98
50	ATOM	2483	C	GLN	B	375	-0.259	12.630	21.104	1.00	24.52
	ATOM	2484	O	GLN	B	375	0.074	11.451	21.221	1.00	23.56
	ATOM	2485	N	VAL	B	376	-1.426	13.013	20.599	1.00	21.87
	ATOM	2486	CA	VAL	B	376	-2.409	12.055	20.140	1.00	23.44
	ATOM	2487	CB	VAL	B	376	-3.718	12.760	19.717	1.00	22.09
55	ATOM	2488	CG1	VAL	B	376	-4.572	11.823	18.877	1.00	24.14
	ATOM	2489	CG2	VAL	B	376	-4.486	13.192	20.954	1.00	16.96
	ATOM	2490	C	VAL	B	376	-1.852	11.257	18.965	1.00	24.15
	ATOM	2491	O	VAL	B	376	-1.949	10.032	18.938	1.00	22.26
	ATOM	2492	N	HIS	B	377	-1.251	11.953	18.007	1.00	25.85
60	ATOM	2493	CA	HIS	B	377	-0.689	11.284	16.843	1.00	25.68
	ATOM	2494	CB	HIS	B	377	-0.078	12.306	15.886	1.00	25.27

5	ATOM	2495	CG	HIS	B	377	0.535	11.690	14.667	1.00	30.63
	ATOM	2496	CD2	HIS	B	377	1.828	11.559	14.287	1.00	31.03
	ATOM	2497	ND1	HIS	B	377	-0.217	11.086	13.683	1.00	35.05
	ATOM	2498	CE1	HIS	B	377	0.588	10.607	12.750	1.00	33.12
	ATOM	2499	NE2	HIS	B	377	1.833	10.882	13.093	1.00	31.06
10	ATOM	2500	C	HIS	B	377	0.365	10.237	17.210	1.00	24.37
	ATOM	2501	O	HIS	B	377	0.321	9.109	16.719	1.00	21.47
	ATOM	2502	N	LEU	B	378	1.307	10.609	18.072	1.00	19.24
	ATOM	2503	CA	LEU	B	378	2.365	9.691	18.474	1.00	20.09
	ATOM	2504	CB	LEU	B	378	3.363	10.402	19.388	1.00	18.64
15	ATOM	2505	CG	LEU	B	378	4.230	11.489	18.736	1.00	22.15
	ATOM	2506	CD1	LEU	B	378	5.104	12.148	19.796	1.00	22.51
	ATOM	2507	CD2	LEU	B	378	5.094	10.885	17.638	1.00	20.68
	ATOM	2508	C	LEU	B	378	1.832	8.433	19.161	1.00	18.91
	ATOM	2509	O	LEU	B	378	2.262	7.320	18.859	1.00	17.52
20	ATOM	2510	N	LEU	B	379	0.888	8.610	20.077	1.00	18.25
	ATOM	2511	CA	LEU	B	379	0.317	7.486	20.795	1.00	18.60
	ATOM	2512	CB	LEU	B	379	-0.526	7.989	21.968	1.00	16.77
	ATOM	2513	CG	LEU	B	379	0.292	8.353	23.214	1.00	17.90
	ATOM	2514	CD1	LEU	B	379	-0.578	9.092	24.211	1.00	15.84
25	ATOM	2515	CD2	LEU	B	379	0.851	7.075	23.842	1.00	22.09
	ATOM	2516	C	LEU	B	379	-0.518	6.605	19.872	1.00	20.17
	ATOM	2517	O	LEU	B	379	-0.476	5.377	19.968	1.00	18.11
	ATOM	2518	N	GLU	B	380	-1.273	7.222	18.971	1.00	19.40
	ATOM	2519	CA	GLU	B	380	-2.086	6.435	18.049	1.00	20.19
30	ATOM	2520	CB	GLU	B	380	-2.994	7.350	17.222	1.00	22.43
	ATOM	2521	CG	GLU	B	380	-4.182	7.874	18.007	1.00	25.30
	ATOM	2522	CD	GLU	B	380	-5.070	8.789	17.188	1.00	29.44
	ATOM	2523	OE1	GLU	B	380	-6.206	9.066	17.625	1.00	31.70
	ATOM	2524	OE2	GLU	B	380	-4.631	9.230	16.110	1.00	31.75
35	ATOM	2525	C	GLU	B	380	-1.210	5.594	17.117	1.00	18.92
	ATOM	2526	O	GLU	B	380	-1.586	4.491	16.722	1.00	19.83
	ATOM	2527	N	ACYS	B	381	-0.039	6.113	16.772	0.75	17.41
	ATOM	2528	N	BCYS	B	381	-0.035	6.113	16.779	0.25	17.76
	ATOM	2529	CA	ACYS	B	381	0.860	5.384	15.887	0.75	20.19
40	ATOM	2530	CA	BCYS	B	381	0.875	5.407	15.884	0.25	17.50
	ATOM	2531	CB	ACYS	B	381	1.870	6.342	15.248	0.75	24.20
	ATOM	2532	CB	BCYS	B	381	1.830	6.406	15.226	0.25	16.63
	ATOM	2533	SG	ACYS	B	381	1.167	7.518	14.060	0.75	33.54
	ATOM	2534	SG	BCYS	B	381	3.048	5.656	14.128	0.25	10.36
45	ATOM	2535	C	ACYS	B	381	1.626	4.269	16.592	0.75	20.59
	ATOM	2536	C	BCYS	B	381	1.689	4.305	16.561	0.25	19.19
	ATOM	2537	O	ACYS	B	381	1.737	3.161	16.069	0.75	19.16
	ATOM	2538	O	BCYS	B	381	1.904	3.241	15.982	0.25	19.25
	ATOM	2539	N	ALA	B	382	2.134	4.560	17.785	1.00	19.04
50	ATOM	2540	CA	ALA	B	382	2.955	3.602	18.530	1.00	20.27
	ATOM	2541	CB	ALA	B	382	4.135	4.364	19.143	1.00	18.68
	ATOM	2542	C	ALA	B	382	2.356	2.702	19.607	1.00	16.82
	ATOM	2543	O	ALA	B	382	3.070	1.852	20.142	1.00	13.37
	ATOM	2544	N	TRP	B	383	1.074	2.855	19.916	1.00	15.30
55	ATOM	2545	CA	TRP	B	383	0.487	2.089	21.013	1.00	15.80
	ATOM	2546	CB	TRP	B	383	-1.009	2.410	21.160	1.00	16.63
	ATOM	2547	CG	TRP	B	383	-1.871	1.775	20.129	1.00	19.93
	ATOM	2548	CD2	TRP	B	383	-2.493	0.483	20.198	1.00	20.80
	ATOM	2549	CE2	TRP	B	383	-3.226	0.309	19.003	1.00	19.27
60	ATOM	2550	CE3	TRP	B	383	-2.506	-0.542	21.155	1.00	21.32
	ATOM	2551	CD1	TRP	B	383	-2.236	2.312	18.933	1.00	18.59

5	ATOM	2552	NE1	TRP	B	383	-3.051	1.439	18.250	1.00	23.67
	ATOM	2553	CZ2	TRP	B	383	-3.963	-0.853	18.733	1.00	21.55
	ATOM	2554	CZ3	TRP	B	383	-3.243	-1.702	20.888	1.00	20.29
	ATOM	2555	CH2	TRP	B	383	-3.960	-1.844	19.686	1.00	19.03
	ATOM	2556	C	TRP	B	383	0.701	0.579	21.020	1.00	17.35
10	ATOM	2557	O	TRP	B	383	0.982	0.010	22.077	1.00	13.92
	ATOM	2558	N	LEU	B	384	0.568	-0.087	19.879	1.00	14.07
	ATOM	2559	CA	LEU	B	384	0.773	-1.532	19.903	1.00	15.98
	ATOM	2560	CB	LEU	B	384	0.181	-2.200	18.656	1.00	12.19
	ATOM	2561	CG	LEU	B	384	0.173	-3.735	18.720	1.00	12.97
15	ATOM	2562	CD1	LEU	B	384	-0.352	-4.240	20.089	1.00	10.65
	ATOM	2563	CD2	LEU	B	384	-0.707	-4.259	17.586	1.00	17.84
	ATOM	2564	C	LEU	B	384	2.262	-1.861	20.034	1.00	14.64
	ATOM	2565	O	LEU	B	384	2.627	-2.833	20.690	1.00	13.78
	ATOM	2566	N	GLU	B	385	3.116	-1.046	19.414	1.00	14.96
20	ATOM	2567	CA	GLU	B	385	4.565	-1.260	19.509	1.00	13.79
	ATOM	2568	CB	GLU	B	385	5.336	-0.179	18.739	1.00	15.34
	ATOM	2569	CG	GLU	B	385	5.297	-0.312	17.207	1.00	15.38
	ATOM	2570	CD	GLU	B	385	6.162	0.738	16.520	1.00	23.97
	ATOM	2571	OE1	GLU	B	385	7.381	0.500	16.358	1.00	21.03
25	ATOM	2572	OE2	GLU	B	385	5.622	1.808	16.149	1.00	22.19
	ATOM	2573	C	GLU	B	385	4.963	-1.161	20.987	1.00	15.79
	ATOM	2574	O	GLU	B	385	5.788	-1.942	21.463	1.00	15.04
	ATOM	2575	N	ILE	B	386	4.389	-0.213	21.690	1.00	13.32
	ATOM	2576	CA	ILE	B	386	4.723	-0.019	23.108	1.00	14.06
30	ATOM	2577	CB	ILE	B	386	4.173	1.326	23.614	1.00	15.36
	ATOM	2578	CG2	ILE	B	386	4.374	1.451	25.130	1.00	15.97
	ATOM	2579	CG1	ILE	B	386	4.910	2.476	22.907	1.00	17.95
	ATOM	2580	CD1	ILE	B	386	4.118	3.768	22.874	1.00	21.12
	ATOM	2581	C	ILE	B	386	4.227	-1.164	23.993	1.00	14.97
35	ATOM	2582	O	ILE	B	386	4.905	-1.560	24.941	1.00	19.60
	ATOM	2583	N	LEU	B	387	3.038	-1.675	23.709	1.00	15.18
	ATOM	2584	CA	LEU	B	387	2.516	-2.791	24.478	1.00	15.98
	ATOM	2585	CB	LEU	B	387	1.070	-3.097	24.080	1.00	17.15
	ATOM	2586	CG	LEU	B	387	-0.031	-2.113	24.486	1.00	19.65
40	ATOM	2587	CD1	LEU	B	387	-1.371	-2.628	23.972	1.00	17.77
	ATOM	2588	CD2	LEU	B	387	-0.075	-1.966	26.002	1.00	15.38
	ATOM	2589	C	LEU	B	387	3.391	-4.013	24.180	1.00	14.69
	ATOM	2590	O	LEU	B	387	3.712	-4.792	25.076	1.00	14.03
	ATOM	2591	N	MET	B	388	3.785	-4.178	22.921	1.00	16.43
45	ATOM	2592	CA	MET	B	388	4.602	-5.329	22.547	1.00	16.67
	ATOM	2593	CB	MET	B	388	4.673	-5.460	21.026	1.00	14.83
	ATOM	2594	CG	MET	B	388	3.403	-6.066	20.453	1.00	13.91
	ATOM	2595	SD	MET	B	388	3.364	-6.193	18.675	1.00	17.23
	ATOM	2596	CE	MET	B	388	1.906	-7.225	18.511	1.00	14.97
50	ATOM	2597	C	MET	B	388	6.004	-5.332	23.133	1.00	20.19
	ATOM	2598	O	MET	B	388	6.460	-6.366	23.636	1.00	21.50
	ATOM	2599	N	ILE	B	389	6.707	-4.203	23.074	1.00	15.34
	ATOM	2600	CA	ILE	B	389	8.044	-4.209	23.634	1.00	15.59
	ATOM	2601	CB	ILE	B	389	8.836	-2.911	23.322	1.00	14.95
55	ATOM	2602	CG2	ILE	B	389	8.330	-1.746	24.158	1.00	12.81
	ATOM	2603	CG1	ILE	B	389	10.325	-3.164	23.602	1.00	17.24
	ATOM	2604	CD1	ILE	B	389	11.228	-1.972	23.357	1.00	15.65
	ATOM	2605	C	ILE	B	389	7.950	-4.446	25.147	1.00	14.30
	ATOM	2606	O	ILE	B	389	8.844	-5.044	25.739	1.00	18.72
60	ATOM	2607	N	GLY	B	390	6.855	-4.007	25.761	1.00	13.99
	ATOM	2608	CA	GLY	B	390	6.681	-4.219	27.189	1.00	14.87

5	ATOM	2609	C	GLY	B	390	6.444	-5.702	27.463	1.00	18.54
	ATOM	2610	O	GLY	B	390	6.989	-6.282	28.403	1.00	16.54
	ATOM	2611	N	LEU	B	391	5.623	-6.325	26.628	1.00	16.15
	ATOM	2612	CA	LEU	B	391	5.334	-7.743	26.775	1.00	18.91
10	ATOM	2613	CB	LEU	B	391	4.332	-8.179	25.699	1.00	19.55
	ATOM	2614	CG	LEU	B	391	4.157	-9.689	25.457	1.00	20.91
	ATOM	2615	CD1	LEU	B	391	3.580	-10.351	26.699	1.00	19.41
	ATOM	2616	CD2	LEU	B	391	3.232	-9.913	24.268	1.00	20.70
15	ATOM	2617	C	LEU	B	391	6.649	-8.518	26.625	1.00	20.31
	ATOM	2618	O	LEU	B	391	7.002	-9.352	27.465	1.00	18.66
	ATOM	2619	N	VAL	B	392	7.378	-8.215	25.557	1.00	18.71
	ATOM	2620	CA	VAL	B	392	8.649	-8.868	25.278	1.00	19.51
20	ATOM	2621	CB	VAL	B	392	9.288	-8.281	24.005	1.00	23.77
	ATOM	2622	CG1	VAL	B	392	10.751	-8.687	23.920	1.00	24.63
	ATOM	2623	CG2	VAL	B	392	8.520	-8.773	22.767	1.00	19.94
	ATOM	2624	C	VAL	B	392	9.615	-8.707	26.450	1.00	22.80
25	ATOM	2625	O	VAL	B	392	10.336	-9.637	26.811	1.00	19.36
	ATOM	2626	N	TRP	B	393	9.617	-7.522	27.046	1.00	22.10
	ATOM	2627	CA	TRP	B	393	10.492	-7.241	28.171	1.00	23.20
	ATOM	2628	CB	TRP	B	393	10.388	-5.773	28.578	1.00	19.22
30	ATOM	2629	CG	TRP	B	393	11.056	-5.479	29.895	1.00	22.53
	ATOM	2630	CD2	TRP	B	393	12.453	-5.591	30.193	1.00	20.36
	ATOM	2631	CE2	TRP	B	393	12.624	-5.208	31.545	1.00	25.65
	ATOM	2632	CE3	TRP	B	393	13.578	-5.976	29.449	1.00	22.12
35	ATOM	2633	CD1	TRP	B	393	10.452	-5.046	31.044	1.00	23.02
	ATOM	2634	NE1	TRP	B	393	11.387	-4.881	32.037	1.00	24.91
	ATOM	2635	CZ2	TRP	B	393	11.387	-5.200	32.171	1.00	23.00
	ATOM	2636	CZ3	TRP	B	393	14.829	-5.968	30.072	1.00	23.98
40	ATOM	2637	CH2	TRP	B	393	14.964	-5.582	31.423	1.00	23.20
	ATOM	2638	C	TRP	B	393	10.208	-8.114	29.388	1.00	24.36
	ATOM	2639	O	TRP	B	393	11.128	-8.717	29.944	1.00	23.04
	ATOM	2640	N	ARG	B	394	8.952	-8.189	29.819	1.00	21.29
45	ATOM	2641	CA	ARG	B	394	8.680	-9.003	30.990	1.00	22.43
	ATOM	2642	CB	ARG	B	394	7.365	-8.601	31.667	1.00	23.97
	ATOM	2643	CG	ARG	B	394	6.259	-8.149	30.759	1.00	26.16
	ATOM	2644	CD	ARG	B	394	5.026	-7.727	31.574	1.00	20.86
50	ATOM	2645	NE	ARG	B	394	3.817	-7.937	30.786	1.00	19.54
	ATOM	2646	CZ	ARG	B	394	3.327	-7.059	29.915	1.00	20.58
	ATOM	2647	NH1	ARG	B	394	3.944	-5.902	29.722	1.00	17.41
	ATOM	2648	NH2	ARG	B	394	2.229	-7.347	29.220	1.00	16.82
55	ATOM	2649	C	ARG	B	394	8.695	-10.502	30.713	1.00	21.78
	ATOM	2650	O	ARG	B	394	8.657	-11.294	31.648	1.00	23.44
	ATOM	2651	N	SER	B	395	8.767	-10.880	29.438	1.00	17.10
	ATOM	2652	CA	SER	B	395	8.805	-12.289	29.041	1.00	25.08
60	ATOM	2653	CB	SER	B	395	8.206	-12.473	27.638	1.00	19.47
	ATOM	2654	OG	SER	B	395	6.832	-12.136	27.619	1.00	21.73
	ATOM	2655	C	SER	B	395	10.239	-12.831	29.031	1.00	26.29
	ATOM	2656	O	SER	B	395	10.458	-14.030	28.854	1.00	23.75
65	ATOM	2657	N	MET	B	396	11.206	-11.938	29.210	1.00	30.79
	ATOM	2658	CA	MET	B	396	12.620	-12.307	29.205	1.00	35.07
	ATOM	2659	CB	MET	B	396	13.479	-11.063	29.423	1.00	33.84
	ATOM	2660	CG	MET	B	396	14.155	-10.569	28.171	1.00	36.88
70	ATOM	2661	SD	MET	B	396	15.149	-9.127	28.491	1.00	40.96
	ATOM	2662	CE	MET	B	396	16.675	-9.849	28.998	1.00	39.67
	ATOM	2663	C	MET	B	396	12.983	-13.353	30.250	1.00	35.88
	ATOM	2664	O	MET	B	396	13.828	-14.215	30.011	1.00	34.52
75	ATOM	2665	N	GLU	B	397	12.348	-13.266	31.410	1.00	36.19

5	ATOM	2666	CA	GLU	B	397	12.604	<del>12.208</del>	32.492	1.00	39.24
	ATOM	2667	CB	GLU	B	397	12.153	-13.605	33.821	1.00	44.38
	ATOM	2668	CG	GLU	B	397	12.983	-12.422	34.271	1.00	54.05
	ATOM	2669	CD	GLU	B	397	13.483	-12.587	35.686	1.00	56.78
	ATOM	2670	OE1	GLU	B	397	13.380	-11.621	36.470	1.00	60.90
10	ATOM	2671	OE2	GLU	B	397	13.975	-13.688	36.013	1.00	60.82
	ATOM	2672	C	GLU	B	397	11.878	-15.528	32.273	1.00	36.65
	ATOM	2673	O	GLU	B	397	12.021	-16.459	33.061	1.00	35.84
	ATOM	2674	N	HIS	B	398	11.100	-15.609	31.202	1.00	32.14
	ATOM	2675	CA	HIS	B	398	10.347	-16.823	30.914	1.00	29.48
15	ATOM	2676	CB	HIS	B	398	8.863	-16.567	31.178	1.00	29.87
	ATOM	2677	CG	HIS	B	398	8.582	-16.111	32.574	1.00	31.80
	ATOM	2678	CD2	HIS	B	398	8.215	-16.801	33.678	1.00	29.12
	ATOM	2679	ND1	HIS	B	398	8.727	-14.799	32.972	1.00	33.27
	ATOM	2680	CE1	HIS	B	398	8.462	-14.701	34.262	1.00	32.19
20	ATOM	2681	NE2	HIS	B	398	8.148	-15.902	34.714	1.00	33.48
	ATOM	2682	C	HIS	B	398	10.556	-17.317	29.492	1.00	25.95
	ATOM	2683	O	HIS	B	398	9.637	-17.291	28.672	1.00	27.47
	ATOM	2684	N	PRO	B	399	11.771	-17.801	29.186	1.00	29.09
	ATOM	2685	CD	PRO	B	399	12.926	-17.922	30.096	1.00	29.93
25	ATOM	2686	CA	PRO	B	399	12.079	-18.300	27.845	1.00	27.40
	ATOM	2687	CB	PRO	B	399	13.434	-18.988	28.016	1.00	32.09
	ATOM	2688	CG	PRO	B	399	14.062	-18.284	29.170	1.00	30.81
	ATOM	2689	C	PRO	B	399	11.009	-19.246	27.319	1.00	29.76
	ATOM	2690	O	PRO	B	399	10.552	-20.137	28.035	1.00	29.18
30	ATOM	2691	N	GLY	B	400	10.601	-19.035	26.071	1.00	27.45
	ATOM	2692	CA	GLY	B	400	9.588	-19.884	25.466	1.00	26.93
	ATOM	2693	C	GLY	B	400	8.161	-19.537	25.849	1.00	26.73
	ATOM	2694	O	GLY	B	400	7.220	-20.153	25.356	1.00	28.36
	ATOM	2695	N	LYS	B	401	7.996	-18.554	26.727	1.00	25.50
35	ATOM	2696	CA	LYS	B	401	6.668	-18.139	27.165	1.00	23.45
	ATOM	2697	CB	LYS	B	401	6.435	-18.563	28.619	1.00	28.50
	ATOM	2698	CG	LYS	B	401	6.476	-20.069	28.879	1.00	28.58
	ATOM	2699	CD	LYS	B	401	6.181	-20.353	30.349	1.00	35.47
	ATOM	2700	CE	LYS	B	401	6.073	-21.847	30.635	1.00	38.59
40	ATOM	2701	NZ	LYS	B	401	7.177	-22.611	29.989	1.00	42.39
	ATOM	2702	C	LYS	B	401	6.493	-16.622	27.060	1.00	21.78
	ATOM	2703	O	LYS	B	401	7.465	-15.872	27.035	1.00	21.45
	ATOM	2704	N	LEU	B	402	5.241	-16.181	26.995	1.00	23.45
	ATOM	2705	CA	LEU	B	402	4.929	-14.759	26.925	1.00	21.37
45	ATOM	2706	CB	LEU	B	402	4.088	-14.449	25.689	1.00	18.47
	ATOM	2707	CG	LEU	B	402	4.798	-14.673	24.360	1.00	16.89
	ATOM	2708	CD1	LEU	B	402	3.821	-14.395	23.211	1.00	21.23
	ATOM	2709	CD2	LEU	B	402	6.011	-13.760	24.277	1.00	23.15
	ATOM	2710	C	LEU	B	402	4.147	-14.399	28.179	1.00	19.66
50	ATOM	2711	O	LEU	B	402	3.024	-14.880	28.381	1.00	18.05
	ATOM	2712	N	LEU	B	403	4.743	-13.559	29.019	1.00	19.54
	ATOM	2713	CA	LEU	B	403	4.099	-13.148	30.259	1.00	20.21
	ATOM	2714	CB	LEU	B	403	5.155	-12.856	31.332	1.00	23.16
	ATOM	2715	CG	LEU	B	403	4.639	-12.682	32.766	1.00	29.54
55	ATOM	2716	CD1	LEU	B	403	5.519	-13.450	33.728	1.00	32.67
	ATOM	2717	CD2	LEU	B	403	4.626	-11.213	33.138	1.00	32.38
	ATOM	2718	C	LEU	B	403	3.219	-11.918	30.043	1.00	20.42
	ATOM	2719	O	LEU	B	403	3.638	-10.787	30.291	1.00	19.18
	ATOM	2720	N	PHE	B	404	2.003	-12.145	29.565	1.00	21.44
60	ATOM	2721	CA	PHE	B	404	1.066	-11.053	29.340	1.00	21.69
	ATOM	2722	CB	PHE	B	404	-0.199	-11.598	28.687	1.00	17.26

5	ATOM	2723	CG	PHE	B	404	-0.026	-11.897	27.227	1.00	19.75
	ATOM	2724	CD1	PHE	B	404	0.364	-13.167	26.801	1.00	17.90
	ATOM	2725	CD2	PHE	B	404	-0.210	-10.897	26.280	1.00	17.04
10	ATOM	2726	CE1	PHE	B	404	0.572	-13.434	25.447	1.00	19.88
	ATOM	2727	CE2	PHE	B	404	-0.007	-11.148	24.924	1.00	18.47
	ATOM	2728	CZ	PHE	B	404	0.386	-12.418	24.503	1.00	16.45
	ATOM	2729	C	PHE	B	404	0.768	-10.403	30.685	1.00	21.95
	ATOM	2730	O	PHE	B	404	0.656	-9.177	30.804	1.00	22.99
15	ATOM	2731	N	ALA	B	405	0.670	-11.247	31.702	1.00	21.12
	ATOM	2732	CA	ALA	B	405	0.424	-10.814	33.066	1.00	22.43
	ATOM	2733	CB	ALA	B	405	-1.074	-10.603	33.304	1.00	24.69
	ATOM	2734	C	ALA	B	405	0.959	-11.926	33.962	1.00	22.40
	ATOM	2735	O	ALA	B	405	1.133	-13.061	33.517	1.00	21.67
20	ATOM	2736	N	PRO	B	406	1.246	-11.612	35.230	1.00	25.60
	ATOM	2737	CD	PRO	B	406	1.129	-10.294	35.878	1.00	23.65
	ATOM	2738	CA	PRO	B	406	1.765	-12.632	36.148	1.00	25.91
	ATOM	2739	CB	PRO	B	406	1.899	-11.882	37.475	1.00	27.04
	ATOM	2740	CG	PRO	B	406	2.017	-10.431	37.068	1.00	26.56
25	ATOM	2741	C	PRO	B	406	0.876	-13.873	36.259	1.00	25.12
	ATOM	2742	O	PRO	B	406	1.368	-14.967	36.538	1.00	28.92
	ATOM	2743	N	ASN	B	407	-0.426	-13.713	36.039	1.00	23.53
	ATOM	2744	CA	ASN	B	407	-1.345	-14.852	36.109	1.00	24.09
	ATOM	2745	CB	ASN	B	407	-2.553	-14.526	36.986	1.00	24.08
30	ATOM	2746	CG	ASN	B	407	-3.327	-13.328	36.486	1.00	26.72
	ATOM	2747	OD1	ASN	B	407	-2.851	-12.574	35.635	1.00	22.65
	ATOM	2748	ND2	ASN	B	407	-4.528	-13.140	37.019	1.00	26.46
	ATOM	2749	C	ASN	B	407	-1.820	-15.231	34.714	1.00	26.91
	ATOM	2750	O	ASN	B	407	-2.859	-15.870	34.548	1.00	28.68
35	ATOM	2751	N	LEU	B	408	-1.059	-14.816	33.708	1.00	27.28
	ATOM	2752	CA	LEU	B	408	-1.387	-15.124	32.327	1.00	27.23
	ATOM	2753	CB	LEU	B	408	-2.247	-14.030	31.699	1.00	26.61
	ATOM	2754	CG	LEU	B	408	-2.815	-14.464	30.341	1.00	27.51
	ATOM	2755	CD1	LEU	B	408	-3.702	-15.692	30.546	1.00	28.75
40	ATOM	2756	CD2	LEU	B	408	-3.598	-13.330	29.694	1.00	25.48
	ATOM	2757	C	LEU	B	408	-0.113	-15.316	31.514	1.00	27.56
	ATOM	2758	O	LEU	B	408	0.247	-14.465	30.695	1.00	26.86
	ATOM	2759	N	LEU	B	409	0.553	-16.426	31.759	1.00	27.54
	ATOM	2760	CA	LEU	B	409	1.786	-16.774	31.065	1.00	31.96
45	ATOM	2761	CB	LEU	B	409	2.786	-17.355	32.058	1.00	31.88
	ATOM	2762	CG	LEU	B	409	4.186	-17.703	31.562	1.00	37.72
	ATOM	2763	CD1	LEU	B	409	4.773	-16.551	30.770	1.00	39.57
	ATOM	2764	CD2	LEU	B	409	5.066	-18.018	32.758	1.00	41.72
	ATOM	2765	C	LEU	B	409	1.401	-17.805	30.009	1.00	31.53
50	ATOM	2766	O	LEU	B	409	0.921	-18.892	30.340	1.00	32.67
	ATOM	2767	N	LEU	B	410	1.604	-17.465	28.746	1.00	29.58
	ATOM	2768	CA	LEU	B	410	1.228	-18.361	27.660	1.00	31.55
	ATOM	2769	CB	LEU	B	410	0.192	-17.672	26.762	1.00	29.83
	ATOM	2770	CG	LEU	B	410	-1.047	-17.080	27.452	1.00	28.55
55	ATOM	2771	CD1	LEU	B	410	-1.770	-16.135	26.501	1.00	26.92
	ATOM	2772	CD2	LEU	B	410	-1.979	-18.200	27.891	1.00	30.49
	ATOM	2773	C	LEU	B	410	2.397	-18.839	26.814	1.00	33.88
	ATOM	2774	O	LEU	B	410	3.427	-18.170	26.726	1.00	36.49
	ATOM	2775	N	ASP	B	411	2.238	-20.013	26.206	1.00	38.80
60	ATOM	2776	CA	ASP	B	411	3.275	-20.562	25.336	1.00	38.39
	ATOM	2777	CB	ASP	B	411	3.657	-21.990	25.752	1.00	44.53
	ATOM	2778	CG	ASP	B	411	2.476	-22.943	25.749	1.00	44.90
	ATOM	2779	OD1	ASP	B	411	1.773	-23.035	24.719	1.00	45.70



5	ATOM	2780	OD2	ASP	B	411	2.254	-23.603	26.786	1.00	50.54
	ATOM	2781	C	ASP	B	411	2.745	-20.551	23.909	1.00	38.57
	ATOM	2782	O	ASP	B	411	1.549	-20.341	23.686	1.00	36.48
	ATOM	2783	N	ARG	B	412	3.635	-20.777	22.949	1.00	36.85
	ATOM	2784	CA	ARG	B	412	3.259	-20.763	21.541	1.00	38.32
10	ATOM	2785	CB	ARG	B	412	4.488	-21.083	20.675	1.00	38.69
	ATOM	2786	CG	ARG	B	412	4.361	-22.314	19.799	1.00	40.05
	ATOM	2787	CD	ARG	B	412	5.644	-22.552	19.012	1.00	42.98
	ATOM	2788	NE	ARG	B	412	5.540	-22.099	17.626	1.00	40.95
	ATOM	2789	CZ	ARG	B	412	4.649	-22.559	16.753	1.00	41.11
15	ATOM	2790	NH1	ARG	B	412	3.777	-23.490	17.115	1.00	44.01
	ATOM	2791	NH2	ARG	B	412	4.632	-22.091	15.515	1.00	41.28
	ATOM	2792	C	ARG	B	412	2.107	-21.712	21.217	1.00	37.64
	ATOM	2793	O	ARG	B	412	1.287	-21.427	20.343	1.00	36.51
	ATOM	2794	N	ASN	B	413	2.041	-22.834	21.923	1.00	35.32
20	ATOM	2795	CA	ASN	B	413	0.974	-23.798	21.688	1.00	36.68
	ATOM	2796	CB	ASN	B	413	1.170	-25.035	22.570	1.00	37.54
	ATOM	2797	CG	ASN	B	413	2.017	-26.100	21.901	1.00	43.56
	ATOM	2798	OD1	ASN	B	413	2.309	-26.022	20.704	1.00	46.11
	ATOM	2799	ND2	ASN	B	413	2.418	-27.104	22.671	1.00	47.04
25	ATOM	2800	C	ASN	B	413	-0.383	-23.168	21.982	1.00	34.01
	ATOM	2801	O	ASN	B	413	-1.349	-23.372	21.247	1.00	32.43
	ATOM	2802	N	GLN	B	414	-0.447	-22.397	23.063	1.00	32.85
	ATOM	2803	CA	GLN	B	414	-1.685	-21.741	23.449	1.00	31.91
	ATOM	2804	CB	GLN	B	414	-1.558	-21.172	24.863	1.00	33.17
30	ATOM	2805	CG	GLN	B	414	-1.528	-22.242	25.948	1.00	32.31
	ATOM	2806	CD	GLN	B	414	-1.293	-21.667	27.327	1.00	34.63
	ATOM	2807	OE1	GLN	B	414	-0.176	-21.277	27.666	1.00	33.23
	ATOM	2808	NE2	GLN	B	414	-2.349	-21.606	28.131	1.00	34.56
	ATOM	2809	C	GLN	B	414	-2.052	-20.638	22.463	1.00	29.57
35	ATOM	2810	O	GLN	B	414	-3.195	-20.204	22.409	1.00	31.32
	ATOM	2811	N	GLY	B	415	-1.077	-20.190	21.682	1.00	30.96
	ATOM	2812	CA	GLY	B	415	-1.350	-19.160	20.697	1.00	34.27
	ATOM	2813	C	GLY	B	415	-2.184	-19.725	19.562	1.00	35.27
	ATOM	2814	O	GLY	B	415	-2.918	-19.000	18.887	1.00	33.20
40	ATOM	2815	N	LYS	B	416	-2.070	-21.031	19.354	1.00	35.28
	ATOM	2816	CA	LYS	B	416	-2.819	-21.707	18.299	1.00	38.26
	ATOM	2817	CB	LYS	B	416	-2.398	-23.177	18.201	1.00	38.00
	ATOM	2818	CG	LYS	B	416	-0.973	-23.407	17.736	1.00	40.05
	ATOM	2819	CD	LYS	B	416	-0.405	-24.668	18.369	1.00	44.10
45	ATOM	2820	CE	LYS	B	416	0.306	-25.541	17.346	1.00	41.85
	ATOM	2821	NZ	LYS	B	416	1.286	-24.760	16.542	1.00	45.63
	ATOM	2822	C	LYS	B	416	-4.321	-21.645	18.559	1.00	36.93
	ATOM	2823	O	LYS	B	416	-5.121	-21.790	17.638	1.00	38.36
	ATOM	2824	N	CYS	B	417	-4.698	-21.430	19.817	1.00	37.10
50	ATOM	2825	CA	CYS	B	417	-6.106	-21.371	20.196	1.00	36.46
	ATOM	2826	CB	CYS	B	417	-6.218	-21.226	21.717	1.00	39.01
	ATOM	2827	SG	CYS	B	417	-5.674	-22.710	22.612	1.00	43.81
	ATOM	2828	C	CYS	B	417	-6.899	-20.277	19.491	1.00	35.19
	ATOM	2829	O	CYS	B	417	-8.127	-20.296	19.485	1.00	33.92
55	ATOM	2830	N	VAL	B	418	-6.195	-19.316	18.906	1.00	36.04
	ATOM	2831	CA	VAL	B	418	-6.838	-18.236	18.163	1.00	34.59
	ATOM	2832	CB	VAL	B	418	-6.525	-16.850	18.775	1.00	34.87
	ATOM	2833	CG1	VAL	B	418	-6.831	-15.763	17.765	1.00	35.32
	ATOM	2834	CG2	VAL	B	418	-7.350	-16.630	20.036	1.00	33.65
60	ATOM	2835	C	VAL	B	418	-6.241	-18.317	16.764	1.00	34.17
	ATOM	2836	O	VAL	B	418	-5.020	-18.323	16.611	1.00	32.73

5	ATOM	2837	N	GLU	B	419	-7.084	-18.388	15.740	1.00	33.44
	ATOM	2838	CA	GLU	B	419	-6.554	-18.500	14.390	1.00	34.52
	ATOM	2839	CB	GLU	B	419	-7.681	-18.722	13.380	1.00	36.21
	ATOM	2840	CG	GLU	B	419	-8.597	-17.538	13.166	1.00	44.19
10	ATOM	2841	CD	GLU	B	419	-9.477	-17.723	11.946	1.00	48.47
	ATOM	2842	OE1	GLU	B	419	-9.157	-18.605	11.119	1.00	51.04
	ATOM	2843	OE2	GLU	B	419	-10.484	-16.993	11.813	1.00	48.91
	ATOM	2844	C	GLU	B	419	-5.717	-17.289	13.997	1.00	32.89
15	ATOM	2845	O	GLU	B	419	-6.156	-16.144	14.123	1.00	31.09
	ATOM	2846	N	GLY	B	420	-4.501	-17.562	13.535	1.00	32.84
	ATOM	2847	CA	GLY	B	420	-3.594	-16.506	13.122	1.00	34.37
	ATOM	2848	C	GLY	B	420	-2.722	-15.955	14.240	1.00	35.30
20	ATOM	2849	O	GLY	B	420	-1.745	-15.246	13.975	1.00	35.94
	ATOM	2850	N	MET	B	421	-3.052	-16.285	15.486	1.00	30.08
	ATOM	2851	CA	MET	B	421	-2.289	-15.780	16.625	1.00	29.22
	ATOM	2852	CB	MET	B	421	-3.108	-15.922	17.914	1.00	22.54
25	ATOM	2853	CG	MET	B	421	-2.469	-15.270	19.124	1.00	23.82
	ATOM	2854	SD	MET	B	421	-2.124	-13.494	18.872	1.00	28.40
	ATOM	2855	CE	MET	B	421	-3.697	-12.800	19.233	1.00	24.67
	ATOM	2856	C	MET	B	421	-0.912	-16.416	16.821	1.00	29.67
30	ATOM	2857	O	MET	B	421	0.022	-15.751	17.269	1.00	29.76
	ATOM	2858	N	VAL	B	422	-0.766	-17.694	16.484	1.00	30.63
	ATOM	2859	CA	VAL	B	422	0.524	-18.338	16.675	1.00	29.90
	ATOM	2860	CB	VAL	B	422	0.482	-19.835	16.273	1.00	35.74
35	ATOM	2861	CG1	VAL	B	422	0.514	-19.992	14.753	1.00	37.64
	ATOM	2862	CG2	VAL	B	422	0.514	-19.992	14.753	1.00	31.68
	ATOM	2863	C	VAL	B	422	1.659	-20.555	16.897	1.00	28.64
	ATOM	2864	O	VAL	B	422	1.669	-17.640	15.935	1.00	26.15
40	ATOM	2865	N	GLU	B	423	2.788	-17.571	16.441	1.00	28.70
	ATOM	2866	CA	GLU	B	423	1.402	-17.113	14.747	1.00	31.34
	ATOM	2867	CB	GLU	B	423	2.454	-16.435	13.997	1.00	36.21
	ATOM	2868	CG	GLU	B	423	1.963	-16.050	12.596	1.00	45.83
45	ATOM	2869	CD	GLU	B	423	0.502	-16.376	12.325	1.00	46.71
	ATOM	2870	OE1	GLU	B	423	0.250	-17.865	12.144	1.00	45.97
	ATOM	2871	OE2	GLU	B	423	-0.746	-18.368	12.706	1.00	50.05
	ATOM	2872	C	GLU	B	423	1.045	-18.530	11.442	1.00	30.57
50	ATOM	2873	O	GLU	B	423	2.928	-15.186	14.744	1.00	26.59
	ATOM	2874	N	ILE	B	424	4.119	-14.870	14.759	1.00	26.19
	ATOM	2875	CA	ILE	B	424	2.001	-14.478	15.378	1.00	26.23
	ATOM	2876	CB	ILE	B	424	2.381	-13.279	16.111	1.00	29.33
55	ATOM	2877	CG2	ILE	B	424	1.134	-12.435	16.452	1.00	30.91
	ATOM	2878	CG1	ILE	B	424	1.492	-11.315	17.425	1.00	29.09
	ATOM	2879	CD1	ILE	B	424	0.584	-11.817	15.160	1.00	30.51
	ATOM	2880	C	ILE	B	424	-0.895	-11.514	15.187	1.00	24.22
60	ATOM	2881	O	ILE	B	424	3.153	-13.673	17.370	1.00	21.05
	ATOM	2882	N	PHE	B	425	4.152	-13.037	17.725	1.00	21.71
	ATOM	2883	CA	PHE	B	425	2.708	-14.746	18.023	1.00	18.85
	ATOM	2884	CB	PHE	B	425	3.370	-15.236	19.223	1.00	22.98
60	ATOM	2885	CG	PHE	B	425	2.650	-16.479	19.768	1.00	22.17
	ATOM	2886	CD1	PHE	B	425	1.580	-16.183	20.795	1.00	25.47
	ATOM	2887	CD2	PHE	B	425	1.287	-17.112	21.792	1.00	26.30
	ATOM	2888	CE1	PHE	B	425	0.843	-15.001	20.747	1.00	24.33
60	ATOM	2889	CE2	PHE	B	425	0.273	-16.871	22.724	1.00	25.03
	ATOM	2890	CZ	PHE	B	425	-0.174	-14.749	21.676	1.00	26.44
	ATOM	2891	C	PHE	B	425	-0.459	-15.684	22.663	1.00	20.00
	ATOM	2892	O	PHE	B	425	4.817	-15.610	18.885	1.00	21.15
60	ATOM	2893	N	ASP	B	426	5.741	-15.292	19.636	1.00	19.87
	ATOM	2893	N	ASP	B	426	5.023	-16.281	17.754	1.00	19.87

5	ATOM	2894	CA	ASP	B	426	6.378	-16.685	17.377	1.00	23.20
	ATOM	2895	CB	ASP	B	426	6.364	-17.510	16.090	1.00	26.53
	ATOM	2896	CG	ASP	B	426	5.992	-18.965	16.335	1.00	34.28
	ATOM	2897	OD1	ASP	B	426	6.242	-19.467	17.455	1.00	35.24
	ATOM	2898	OD2	ASP	B	426	5.448	-19.600	15.409	1.00	31.49
10	ATOM	2899	C	ASP	B	426	7.302	-15.489	17.198	1.00	21.84
	ATOM	2900	O	ASP	B	426	8.465	-15.526	17.593	1.00	21.55
	ATOM	2901	N	MET	B	427	6.788	-14.429	16.591	1.00	20.12
	ATOM	2902	CA	MET	B	427	7.597	-13.234	16.382	1.00	21.02
	ATOM	2903	CB	MET	B	427	6.836	-12.228	15.520	1.00	18.53
15	ATOM	2904	CG	MET	B	427	6.864	-12.559	14.038	1.00	27.92
	ATOM	2905	SD	MET	B	427	6.011	-11.341	13.024	1.00	32.84
	ATOM	2906	CE	MET	B	427	4.363	-11.532	13.581	1.00	33.63
	ATOM	2907	C	MET	B	427	7.945	-12.616	17.732	1.00	17.42
	ATOM	2908	O	MET	B	427	9.073	-12.180	17.950	1.00	22.09
20	ATOM	2909	N	LEU	B	428	6.968	-12.597	18.634	1.00	20.47
	ATOM	2910	CA	LEU	B	428	7.157	-12.033	19.968	1.00	20.13
	ATOM	2911	CB	LEU	B	428	5.812	-11.964	20.706	1.00	17.58
	ATOM	2912	CG	LEU	B	428	4.852	-10.887	20.179	1.00	18.41
	ATOM	2913	CD1	LEU	B	428	3.443	-11.155	20.687	1.00	11.95
25	ATOM	2914	CD2	LEU	B	428	5.324	-9.505	20.631	1.00	17.80
	ATOM	2915	C	LEU	B	428	8.159	-12.856	20.767	1.00	20.68
	ATOM	2916	O	LEU	B	428	9.028	-12.305	21.445	1.00	20.45
	ATOM	2917	N	LEU	B	429	8.037	-14.178	20.679	1.00	20.35
	ATOM	2918	CA	LEU	B	429	8.938	-15.082	21.382	1.00	19.82
30	ATOM	2919	CB	LEU	B	429	8.470	-16.532	21.211	1.00	23.13
	ATOM	2920	CG	LEU	B	429	7.189	-16.839	21.997	1.00	21.85
	ATOM	2921	CD1	LEU	B	429	6.551	-18.123	21.494	1.00	25.39
	ATOM	2922	CD2	LEU	B	429	7.537	-16.944	23.475	1.00	24.91
	ATOM	2923	C	LEU	B	429	10.361	-14.936	20.865	1.00	20.74
35	ATOM	2924	O	LEU	B	429	11.318	-14.968	21.638	1.00	21.02
	ATOM	2925	N	ALA	B	430	10.495	-14.770	19.554	1.00	21.40
	ATOM	2926	CA	ALA	B	430	11.808	-14.609	18.947	1.00	22.77
	ATOM	2927	CB	ALA	B	430	11.677	-14.596	17.432	1.00	21.11
	ATOM	2928	C	ALA	B	430	12.467	-13.315	19.440	1.00	22.40
40	ATOM	2929	O	ALA	B	430	13.670	-13.277	19.713	1.00	20.62
	ATOM	2930	N	THR	B	431	11.670	-12.258	19.567	1.00	21.09
	ATOM	2931	CA	THR	B	431	12.183	-10.974	20.021	1.00	22.67
	ATOM	2932	CB	THR	B	431	11.128	-9.866	19.863	1.00	23.77
	ATOM	2933	OG1	THR	B	431	10.572	-9.936	18.547	1.00	23.84
45	ATOM	2934	CG2	THR	B	431	11.762	-8.489	20.073	1.00	21.78
	ATOM	2935	C	THR	B	431	12.603	-11.037	21.480	1.00	21.98
	ATOM	2936	O	THR	B	431	13.595	-10.429	21.879	1.00	19.85
	ATOM	2937	N	SER	B	432	11.844	-11.773	22.280	1.00	24.24
	ATOM	2938	CA	SER	B	432	12.169	-11.906	23.693	1.00	26.96
50	ATOM	2939	CB	SER	B	432	11.055	-12.661	24.423	1.00	28.00
	ATOM	2940	OG	SER	B	432	11.404	-12.888	25.776	1.00	30.31
	ATOM	2941	C	SER	B	432	13.491	-12.660	23.820	1.00	27.67
	ATOM	2942	O	SER	B	432	14.305	-12.377	24.701	1.00	23.78
	ATOM	2943	N	SER	B	433	13.691	-13.628	22.932	1.00	29.27
55	ATOM	2944	CA	SER	B	433	14.914	-14.421	22.928	1.00	31.96
	ATOM	2945	CB	SER	B	433	14.790	-15.575	21.938	1.00	30.84
	ATOM	2946	OG	SER	B	433	14.761	-16.808	22.625	1.00	38.26
	ATOM	2947	C	SER	B	433	16.104	-13.550	22.548	1.00	31.47
	ATOM	2948	O	SER	B	433	17.204	-13.701	23.087	1.00	28.43
60	ATOM	2949	N	ARG	B	434	15.878	-12.641	21.607	1.00	29.55
	ATOM	2950	CA	ARG	B	434	16.926	-11.739	21.165	1.00	29.40

5	ATOM	2951	CB	ARG	B	434	16.437	-10.912	19.977	1.00	31.56
	ATOM	2952	CG	ARG	B	434	17.428	-9.868	19.493	1.00	36.76
	ATOM	2953	CD	ARG	B	434	18.694	-10.502	18.919	1.00	37.76
	ATOM	2954	NE	ARG	B	434	19.654	-9.479	18.516	1.00	39.50
	ATOM	2955	CZ	ARG	B	434	20.965	-9.673	18.418	1.00	44.17
10	ATOM	2956	NH1	ARG	B	434	21.492	-10.861	18.696	1.00	43.17
	ATOM	2957	NH2	ARG	B	434	21.750	-8.671	18.048	1.00	43.05
	ATOM	2958	C	ARG	B	434	17.328	-10.827	22.326	1.00	29.15
	ATOM	2959	O	ARG	B	434	18.515	-10.612	22.569	1.00	28.82
	ATOM	2960	N	PHE	B	435	16.337	-10.297	23.039	1.00	24.88
15	ATOM	2961	CA	PHE	B	435	16.600	-9.422	24.186	1.00	25.74
	ATOM	2962	CB	PHE	B	435	15.278	-8.972	24.825	1.00	26.53
	ATOM	2963	CG	PHE	B	435	14.656	-7.758	24.183	1.00	30.94
	ATOM	2964	CD1	PHE	B	435	15.118	-7.271	22.966	1.00	32.65
	ATOM	2965	CD2	PHE	B	435	13.592	-7.108	24.797	1.00	33.60
20	ATOM	2966	CE1	PHE	B	435	14.529	-6.155	22.372	1.00	36.84
	ATOM	2967	CE2	PHE	B	435	12.997	-5.989	24.208	1.00	34.96
	ATOM	2968	CZ	PHE	B	435	13.468	-5.516	22.995	1.00	31.64
	ATOM	2969	C	PHE	B	435	17.426	-10.184	25.233	1.00	25.39
	ATOM	2970	O	PHE	B	435	18.414	-9.675	25.764	1.00	22.59
25	ATOM	2971	N	ARG	B	436	16.999	-11.405	25.528	1.00	24.58
	ATOM	2972	CA	ARG	B	436	17.675	-12.253	26.503	1.00	30.25
	ATOM	2973	CB	ARG	B	436	16.898	-13.569	26.662	1.00	33.32
	ATOM	2974	CG	ARG	B	436	17.232	-14.358	27.915	1.00	38.17
	ATOM	2975	CD	ARG	B	436	16.135	-15.367	28.260	1.00	37.27
30	ATOM	2976	NE	ARG	B	436	15.646	-16.085	27.086	1.00	43.92
	ATOM	2977	CZ	ARG	B	436	14.433	-15.923	26.557	1.00	46.68
	ATOM	2978	NH1	ARG	B	436	13.578	-15.061	27.097	1.00	45.59
	ATOM	2979	NH2	ARG	B	436	14.074	-16.620	25.486	1.00	46.25
	ATOM	2980	C	ARG	B	436	19.110	-12.531	26.048	1.00	29.82
35	ATOM	2981	O	ARG	B	436	20.057	-12.397	26.823	1.00	28.76
	ATOM	2982	N	AMET	B	437	19.269	-12.921	24.789	0.50	30.27
	ATOM	2983	N	BMET	B	437	19.252	-12.906	24.781	0.50	31.41
	ATOM	2984	CA	AMET	B	437	20.591	-13.212	24.253	0.50	31.98
	ATOM	2985	CA	BMET	B	437	20.547	-13.206	24.183	0.50	33.77
40	ATOM	2986	CB	AMET	B	437	20.489	-13.646	22.788	0.50	31.34
	ATOM	2987	CB	BMET	B	437	20.348	-13.595	22.714	0.50	35.88
	ATOM	2988	CG	AMET	B	437	20.179	-15.127	22.592	0.50	33.62
	ATOM	2989	CG	BMET	B	437	21.605	-13.594	21.861	0.50	40.47
	ATOM	2990	SD	AMET	B	437	20.354	-16.099	24.109	0.50	35.21
45	ATOM	2991	SD	BMET	B	437	21.247	-13.937	20.115	0.50	46.79
	ATOM	2992	CE	AMET	B	437	22.155	-16.194	24.259	0.50	33.20
	ATOM	2993	CE	BMET	B	437	21.837	-15.632	19.976	0.50	43.22
	ATOM	2994	C	AMET	B	437	21.498	-11.993	24.366	0.50	33.33
	ATOM	2995	C	BMET	B	437	21.487	-12.005	24.289	0.50	34.45
50	ATOM	2996	O	AMET	B	437	22.702	-12.123	24.594	0.50	33.54
	ATOM	2997	O	BMET	B	437	22.699	-12.162	24.438	0.50	34.43
	ATOM	2998	N	MET	B	438	20.913	-10.809	24.215	1.00	32.07
	ATOM	2999	CA	MET	B	438	21.674	-9.560	24.298	1.00	32.48
	ATOM	3000	CB	MET	B	438	20.930	-8.437	23.578	1.00	29.74
55	ATOM	3001	CG	MET	B	438	21.161	-8.364	22.093	1.00	36.73
	ATOM	3002	SD	MET	B	438	20.425	-6.849	21.462	1.00	38.21
	ATOM	3003	CE	MET	B	438	21.693	-5.657	21.943	1.00	35.91
	ATOM	3004	C	MET	B	438	21.877	-9.122	25.738	1.00	28.81
	ATOM	3005	O	MET	B	438	22.686	-8.240	26.013	1.00	30.13
60	ATOM	3006	N	ASN	B	439	21.120	-9.721	26.646	1.00	27.14
	ATOM	3007	CA	ASN	B	439	21.199	-9.359	28.038	1.00	27.34

5	ATOM	3008	CB	ASN	B	439	22.592	-9.524	28.598	1.00	34.85
	ATOM	3009	CG	ASN	B	439	22.624	-9.480	30.080	1.00	38.58
	ATOM	3010	OD1	ASN	B	439	21.584	-9.620	30.724	1.00	42.99
	ATOM	3011	ND2	ASN	B	439	23.801	-9.260	30.666	1.00	41.14
	ATOM	3012	C	ASN	B	439	20.745	-7.903	28.212	1.00	26.24
10	ATOM	3013	O	ASN	B	439	21.396	-7.106	28.891	1.00	19.76
	ATOM	3014	N	LEU	B	440	19.625	-7.564	27.573	1.00	24.90
	ATOM	3015	CA	LEU	B	440	19.061	-6.214	27.633	1.00	25.04
	ATOM	3016	CB	LEU	B	440	17.761	-6.157	26.818	1.00	22.36
	ATOM	3017	CG	LEU	B	440	17.087	-4.786	26.740	1.00	26.33
15	ATOM	3018	CD1	LEU	B	440	17.958	-3.843	25.923	1.00	28.33
	ATOM	3019	CD2	LEU	B	440	15.704	-4.914	26.111	1.00	24.81
	ATOM	3020	C	LEU	B	440	18.782	-5.785	29.074	1.00	24.71
	ATOM	3021	O	LEU	B	440	18.131	-6.504	29.830	1.00	26.96
	ATOM	3022	N	GLN	B	441	19.268	-4.609	29.452	1.00	25.54
20	ATOM	3023	CA	GLN	B	441	19.060	-4.099	30.807	1.00	25.82
	ATOM	3024	CB	GLN	B	441	20.250	-3.231	31.234	1.00	30.41
	ATOM	3025	CG	GLN	B	441	21.572	-3.956	31.228	1.00	30.50
	ATOM	3026	CD	GLN	B	441	21.610	-5.028	32.279	1.00	32.75
	ATOM	3027	OE1	GLN	B	441	21.539	-4.772	33.473	1.00	36.52
25	ATOM	3028	NE2	GLN	B	441	21.703	-6.288	31.823	1.00	31.09
	ATOM	3029	C	GLN	B	441	17.789	-3.265	30.883	1.00	26.93
	ATOM	3030	O	GLN	B	441	17.303	-2.768	29.866	1.00	25.40
	ATOM	3031	N	GLY	B	442	17.266	-3.105	32.096	1.00	24.56
	ATOM	3032	CA	GLY	B	442	16.058	-2.327	32.293	1.00	22.82
30	ATOM	3033	C	GLY	B	442	16.217	-0.873	31.885	1.00	24.19
	ATOM	3034	O	GLY	B	442	15.290	-0.279	31.341	1.00	20.21
	ATOM	3035	N	GLU	B	443	17.387	-0.293	32.141	1.00	22.92
	ATOM	3036	CA	GLU	B	443	17.635	1.102	31.778	1.00	23.33
	ATOM	3037	CB	GLU	B	443	18.960	1.590	32.378	1.00	24.26
35	ATOM	3038	CG	GLU	B	443	19.005	1.525	33.895	1.00	32.31
	ATOM	3039	CD	GLU	B	443	19.701	0.270	34.402	1.00	37.68
	ATOM	3040	OE1	GLU	B	443	19.343	-0.841	33.948	1.00	35.23
	ATOM	3041	OE2	GLU	B	443	20.607	0.394	35.252	1.00	42.47
	ATOM	3042	C	GLU	B	443	17.662	1.278	30.262	1.00	23.08
40	ATOM	3043	O	GLU	B	443	17.265	2.328	29.747	1.00	21.80
	ATOM	3044	N	GLU	B	444	18.128	0.253	29.552	1.00	21.16
	ATOM	3045	CA	GLU	B	444	18.182	0.302	28.093	1.00	22.60
	ATOM	3046	CB	GLU	B	444	19.046	-0.834	27.545	1.00	20.89
	ATOM	3047	CG	GLU	B	444	20.545	-0.617	27.705	1.00	23.24
45	ATOM	3048	CD	GLU	B	444	21.340	-1.869	27.393	1.00	22.11
	ATOM	3049	OE1	GLU	B	444	20.817	-2.978	27.629	1.00	20.89
	ATOM	3050	OE2	GLU	B	444	22.488	-1.746	26.914	1.00	25.49
	ATOM	3051	C	GLU	B	444	16.758	0.155	27.552	1.00	21.06
	ATOM	3052	O	GLU	B	444	16.377	0.822	26.597	1.00	23.73
50	ATOM	3053	N	PHE	B	445	15.987	-0.730	28.176	1.00	19.01
	ATOM	3054	CA	PHE	B	445	14.600	-0.969	27.792	1.00	19.44
	ATOM	3055	CB	PHE	B	445	13.989	-2.067	28.675	1.00	18.12
	ATOM	3056	CG	PHE	B	445	12.483	-2.055	28.709	1.00	18.13
	ATOM	3057	CD1	PHE	B	445	11.746	-2.386	27.575	1.00	18.34
55	ATOM	3058	CD2	PHE	B	445	11.802	-1.694	29.872	1.00	16.59
	ATOM	3059	CE1	PHE	B	445	10.346	-2.359	27.592	1.00	17.15
	ATOM	3060	CE2	PHE	B	445	10.406	-1.662	29.903	1.00	21.99
	ATOM	3061	CZ	PHE	B	445	9.674	-1.997	28.755	1.00	16.01
	ATOM	3062	C	PHE	B	445	13.758	0.304	27.888	1.00	15.87
60	ATOM	3063	O	PHE	B	445	13.008	0.617	26.966	1.00	20.27
	ATOM	3064	N	VAL	B	446	13.872	1.044	28.986	1.00	15.90

5	ATOM	3065	CA	VAL	B	446	13.074	2.269	29.112	1.00	16.78
	ATOM	3066	CB	VAL	B	446	13.165	2.895	30.531	1.00	18.32
	ATOM	3067	CG1	VAL	B	446	12.574	1.923	31.551	1.00	21.14
	ATOM	3068	CG2	VAL	B	446	14.598	3.251	30.879	1.00	21.04
	ATOM	3069	C	VAL	B	446	13.450	3.295	28.051	1.00	17.91
10	ATOM	3070	O	VAL	B	446	12.596	4.028	27.561	1.00	19.37
	ATOM	3071	N	CYS	B	447	14.723	3.335	27.674	1.00	18.81
	ATOM	3072	CA	CYS	B	447	15.161	4.255	26.635	1.00	17.34
	ATOM	3073	CB	CYS	B	447	16.682	4.224	26.512	1.00	19.33
	ATOM	3074	SG	CYS	B	447	17.538	5.134	27.798	1.00	23.60
15	ATOM	3075	C	CYS	B	447	14.537	3.826	25.301	1.00	18.09
	ATOM	3076	O	CYS	B	447	13.988	4.643	24.563	1.00	17.52
	ATOM	3077	N	LEU	B	448	14.623	2.533	25.006	1.00	15.60
	ATOM	3078	CA	LEU	B	448	14.072	1.994	23.767	1.00	16.67
	ATOM	3079	CB	LEU	B	448	14.328	0.490	23.684	1.00	14.82
20	ATOM	3080	CG	LEU	B	448	15.730	0.009	23.301	1.00	23.57
	ATOM	3081	CD1	LEU	B	448	15.722	-1.522	23.169	1.00	21.61
	ATOM	3082	CD2	LEU	B	448	16.167	0.658	21.986	1.00	18.92
	ATOM	3083	C	LEU	B	448	12.573	2.249	23.652	1.00	15.98
	ATOM	3084	O	LEU	B	448	12.078	2.633	22.590	1.00	18.91
25	ATOM	3085	N	LYS	B	449	11.849	2.037	24.745	1.00	17.94
	ATOM	3086	CA	LYS	B	449	10.405	2.232	24.733	1.00	16.66
	ATOM	3087	CB	LYS	B	449	9.796	1.745	26.047	1.00	16.45
	ATOM	3088	CG	LYS	B	449	8.285	1.861	26.115	1.00	16.12
	ATOM	3089	CD	LYS	B	449	7.730	0.952	27.193	1.00	19.09
30	ATOM	3090	CE	LYS	B	449	8.201	1.380	28.580	1.00	17.04
	ATOM	3091	NZ	LYS	B	449	7.159	1.088	29.593	1.00	17.25
	ATOM	3092	C	LYS	B	449	10.058	3.696	24.486	1.00	18.78
	ATOM	3093	O	LYS	B	449	9.103	3.996	23.769	1.00	14.84
	ATOM	3094	N	SER	B	450	10.837	4.610	25.059	1.00	14.50
35	ATOM	3095	CA	SER	B	450	10.591	6.032	24.849	1.00	17.11
	ATOM	3096	CB	SER	B	450	11.440	6.866	25.815	1.00	21.20
	ATOM	3097	OG	SER	B	450	10.859	6.868	27.108	1.00	30.66
	ATOM	3098	C	SER	B	450	10.921	6.418	23.405	1.00	17.84
	ATOM	3099	O	SER	B	450	10.279	7.292	22.821	1.00	18.82
40	ATOM	3100	N	ILE	B	451	11.926	5.768	22.828	1.00	16.88
	ATOM	3101	CA	ILE	B	451	12.305	6.063	21.450	1.00	17.11
	ATOM	3102	CB	ILE	B	451	13.564	5.268	21.025	1.00	16.69
	ATOM	3103	CG2	ILE	B	451	13.724	5.298	19.505	1.00	19.31
	ATOM	3104	CG1	ILE	B	451	14.804	5.897	21.676	1.00	18.96
45	ATOM	3105	CD1	ILE	B	451	16.083	5.130	21.431	1.00	18.98
	ATOM	3106	C	ILE	B	451	11.142	5.711	20.527	1.00	18.09
	ATOM	3107	O	ILE	B	451	10.820	6.464	19.608	1.00	17.07
	ATOM	3108	N	ILE	B	452	10.505	4.571	20.786	1.00	18.13
	ATOM	3109	CA	ILE	B	452	9.373	4.137	19.976	1.00	16.77
50	ATOM	3110	CB	ILE	B	452	8.804	2.775	20.477	1.00	17.40
	ATOM	3111	CG2	ILE	B	452	7.464	2.496	19.831	1.00	14.33
	ATOM	3112	CG1	ILE	B	452	9.763	1.635	20.107	1.00	15.36
	ATOM	3113	CD1	ILE	B	452	9.449	0.323	20.805	1.00	17.76
	ATOM	3114	C	ILE	B	452	8.271	5.195	20.024	1.00	17.47
55	ATOM	3115	O	ILE	B	452	7.733	5.586	18.992	1.00	16.50
	ATOM	3116	N	LEU	B	453	7.943	5.665	21.222	1.00	16.06
	ATOM	3117	CA	LEU	B	453	6.903	6.680	21.374	1.00	17.17
	ATOM	3118	CB	LEU	B	453	6.736	7.061	22.850	1.00	16.23
	ATOM	3119	CG	LEU	B	453	5.792	8.228	23.163	1.00	17.60
60	ATOM	3120	CD1	LEU	B	453	4.388	7.881	22.704	1.00	16.94
	ATOM	3121	CD2	LEU	B	453	5.816	8.538	24.667	1.00	17.17

5	ATOM	3122	C	LEU	B	453	7.198	7.941	20.566	1.00	19.33
	ATOM	3123	O	LEU	B	453	6.320	8.458	19.879	1.00	21.37
	ATOM	3124	N	LEU	B	454	8.434	8.428	20.636	1.00	17.68
	ATOM	3125	CA	LEU	B	454	8.789	9.653	19.933	1.00	20.93
	ATOM	3126	CB	LEU	B	454	9.959	10.347	20.653	1.00	24.33
10	ATOM	3127	CG	LEU	B	454	9.735	10.699	22.130	1.00	26.16
	ATOM	3128	CD1	LEU	B	454	11.046	11.170	22.749	1.00	24.82
	ATOM	3129	CD2	LEU	B	454	8.658	11.777	22.259	1.00	23.79
	ATOM	3130	C	LEU	B	454	9.120	9.494	18.449	1.00	20.75
	ATOM	3131	O	LEU	B	454	8.941	10.431	17.673	1.00	21.33
15	ATOM	3132	N	ASN	B	455	9.566	8.311	18.042	1.00	20.54
	ATOM	3133	CA	ASN	B	455	9.951	8.093	16.651	1.00	19.46
	ATOM	3134	CB	ASN	B	455	11.147	7.149	16.584	1.00	18.58
	ATOM	3135	CG	ASN	B	455	11.576	6.871	15.161	1.00	17.64
	ATOM	3136	OD1	ASN	B	455	12.106	7.749	14.496	1.00	18.40
20	ATOM	3137	ND2	ASN	B	455	11.343	5.648	14.686	1.00	15.06
	ATOM	3138	C	ASN	B	455	8.925	7.580	15.655	1.00	22.77
	ATOM	3139	O	ASN	B	455	8.790	8.127	14.564	1.00	21.94
	ATOM	3140	N	SER	B	456	8.224	6.514	16.023	1.00	25.90
	ATOM	3141	CA	SER	B	456	7.260	5.873	15.135	1.00	24.76
25	ATOM	3142	CB	SER	B	456	6.402	4.894	15.939	1.00	26.91
	ATOM	3143	OG	SER	B	456	7.212	3.818	16.390	1.00	26.24
	ATOM	3144	C	SER	B	456	6.385	6.774	14.272	1.00	26.52
	ATOM	3145	O	SER	B	456	6.323	6.588	13.055	1.00	29.22
	ATOM	3146	N	GLY	B	457	5.716	7.750	14.872	1.00	22.07
30	ATOM	3147	CA	GLY	B	457	4.879	8.627	14.076	1.00	25.19
	ATOM	3148	C	GLY	B	457	5.510	9.973	13.765	1.00	28.59
	ATOM	3149	O	GLY	B	457	4.851	10.850	13.214	1.00	28.31
	ATOM	3150	N	VAL	B	458	6.789	10.130	14.092	1.00	31.65
	ATOM	3151	CA	VAL	B	458	7.486	11.396	13.879	1.00	38.50
35	ATOM	3152	CB	VAL	B	458	8.950	11.310	14.373	1.00	36.24
	ATOM	3153	CG1	VAL	B	458	9.827	10.650	13.324	1.00	38.50
	ATOM	3154	CG2	VAL	B	458	9.463	12.699	14.701	1.00	39.84
	ATOM	3155	C	VAL	B	458	7.483	11.982	12.464	1.00	46.30
	ATOM	3156	O	VAL	B	458	7.567	13.201	12.302	1.00	47.67
40	ATOM	3157	N	TYR	B	459	7.393	11.138	11.442	1.00	50.45
	ATOM	3158	CA	TYR	B	459	7.385	11.640	10.069	1.00	57.07
	ATOM	3159	CB	TYR	B	459	8.233	10.740	9.170	1.00	57.05
	ATOM	3160	CG	TYR	B	459	9.673	10.680	9.611	1.00	59.29
	ATOM	3161	CD1	TYR	B	459	10.284	11.786	10.203	1.00	60.93
45	ATOM	3162	CE1	TYR	B	459	11.591	11.725	10.662	1.00	61.86
	ATOM	3163	CD2	TYR	B	459	10.414	9.510	9.486	1.00	59.46
	ATOM	3164	CE2	TYR	B	459	11.726	9.439	9.943	1.00	59.67
	ATOM	3165	CZ	TYR	B	459	12.305	10.548	10.532	1.00	60.84
	ATOM	3166	OH	TYR	B	459	13.593	10.477	11.009	1.00	61.39
50	ATOM	3167	C	TYR	B	459	5.976	11.753	9.514	1.00	61.22
	ATOM	3168	O	TYR	B	459	5.629	12.750	8.874	1.00	62.89
	ATOM	3169	N	THR	B	460	5.166	10.730	9.768	1.00	65.15
	ATOM	3170	CA	THR	B	460	3.783	10.702	9.309	1.00	67.76
	ATOM	3171	CB	THR	B	460	3.178	9.283	9.464	1.00	68.02
55	ATOM	3172	OG1	THR	B	460	1.890	9.235	8.836	1.00	67.03
	ATOM	3173	CG2	THR	B	460	3.040	8.916	10.938	1.00	67.31
	ATOM	3174	C	THR	B	460	2.945	11.700	10.107	1.00	70.14
	ATOM	3175	O	THR	B	460	1.715	11.641	10.099	1.00	72.35
	ATOM	3176	N	PHE	B	461	3.625	12.620	10.788	1.00	72.64
60	ATOM	3177	CA	PHE	B	461	2.969	13.637	11.607	1.00	75.05
	ATOM	3178	CB	PHE	B	461	3.977	14.720	12.012	1.00	75.47

5	ATOM	3179	CG	PHE	B	461	4.235	14.789	13.492	1.00	74.32
	ATOM	3180	CD1	PHE	B	461	3.200	14.609	14.404	1.00	73.98
	ATOM	3181	CD2	PHE	B	461	5.517	15.025	13.975	1.00	75.22
	ATOM	3182	CE1	PHE	B	461	3.438	14.662	15.775	1.00	74.02
	ATOM	3183	CE2	PHE	B	461	5.765	15.080	15.344	1.00	74.50
10	ATOM	3184	CZ	PHE	B	461	4.722	14.897	16.245	1.00	74.10
	ATOM	3185	C	PHE	B	461	1.787	14.286	10.896	1.00	76.78
	ATOM	3186	O	PHE	B	461	1.775	14.279	9.645	1.00	77.08
	ATOM	3187	CB	GLU	B	470	7.873	23.789	14.718	1.00	80.19
	ATOM	3188	C	GLU	B	470	8.958	21.731	15.650	1.00	79.30
15	ATOM	3189	O	GLU	B	470	9.887	21.518	16.432	1.00	78.21
	ATOM	3190	N	GLU	B	470	9.096	22.235	13.227	1.00	80.22
	ATOM	3191	CA	GLU	B	470	9.060	22.830	14.595	1.00	80.03
	ATOM	3192	N	GLU	B	471	7.823	21.037	15.665	1.00	78.31
	ATOM	3193	CA	GLU	B	471	7.596	19.956	16.617	1.00	75.83
20	ATOM	3194	CB	GLU	B	471	6.118	19.543	16.604	1.00	76.70
	ATOM	3195	CG	GLU	B	471	5.742	18.544	15.516	1.00	78.42
	ATOM	3196	CD	GLU	B	471	5.062	19.198	14.327	1.00	79.69
	ATOM	3197	OE1	GLU	B	471	3.829	19.398	14.378	1.00	80.26
	ATOM	3198	OE2	GLU	B	471	5.763	19.511	13.340	1.00	80.72
25	ATOM	3199	C	GLU	B	471	8.487	18.756	16.292	1.00	73.13
	ATOM	3200	O	GLU	B	471	8.897	18.021	17.189	1.00	73.86
	ATOM	3201	N	LYS	B	472	8.785	18.565	15.009	1.00	69.65
	ATOM	3202	CA	LYS	B	472	9.639	17.461	14.581	1.00	64.40
	ATOM	3203	CB	LYS	B	472	9.578	17.293	13.060	1.00	63.78
30	ATOM	3204	CG	LYS	B	472	8.343	16.552	12.566	1.00	64.49
	ATOM	3205	CD	LYS	B	472	8.544	16.002	11.161	1.00	63.81
	ATOM	3206	CE	LYS	B	472	7.379	16.368	10.249	1.00	64.90
	ATOM	3207	NZ	LYS	B	472	6.475	15.212	9.990	1.00	63.97
	ATOM	3208	C	LYS	B	472	11.071	17.749	15.014	1.00	61.03
35	ATOM	3209	O	LYS	B	472	11.848	16.833	15.287	1.00	60.28
	ATOM	3210	N	ASP	B	473	11.413	19.033	15.076	1.00	56.84
	ATOM	3211	CA	ASP	B	473	12.745	19.451	15.488	1.00	51.69
	ATOM	3212	CB	ASP	B	473	12.923	20.940	15.242	1.00	50.36
	ATOM	3213	C	ASP	B	473	12.923	19.138	16.970	1.00	49.18
40	ATOM	3214	O	ASP	B	473	13.959	18.619	17.385	1.00	46.85
	ATOM	3215	N	HIS	B	474	11.898	19.449	17.758	1.00	45.35
	ATOM	3216	CA	HIS	B	474	11.923	19.203	19.196	1.00	43.65
	ATOM	3217	CB	HIS	B	474	10.652	19.761	19.847	1.00	43.70
	ATOM	3218	CG	HIS	B	474	10.458	19.326	21.267	1.00	43.86
45	ATOM	3219	CD2	HIS	B	474	11.095	19.688	22.406	1.00	44.12
	ATOM	3220	ND1	HIS	B	474	9.510	18.395	21.638	1.00	46.60
	ATOM	3221	CE1	HIS	B	474	9.572	18.202	22.943	1.00	45.29
	ATOM	3222	NE2	HIS	B	474	10.526	18.975	23.434	1.00	47.96
	ATOM	3223	C	HIS	B	474	12.030	17.707	19.471	1.00	42.38
50	ATOM	3224	O	HIS	B	474	12.834	17.273	20.298	1.00	42.83
	ATOM	3225	N	ILE	B	475	11.214	16.923	18.773	1.00	38.86
	ATOM	3226	CA	ILE	B	475	11.222	15.475	18.943	1.00	36.53
	ATOM	3227	CB	ILE	B	475	10.105	14.822	18.110	1.00	36.56
	ATOM	3228	CG2	ILE	B	475	10.390	13.335	17.911	1.00	36.17
55	ATOM	3229	CG1	ILE	B	475	8.770	14.998	18.832	1.00	35.81
	ATOM	3230	CD1	ILE	B	475	7.598	14.410	18.094	1.00	41.77
	ATOM	3231	C	ILE	B	475	12.575	14.898	18.532	1.00	33.72
	ATOM	3232	O	ILE	B	475	13.112	14.023	19.207	1.00	31.50
	ATOM	3233	N	HIS	B	476	13.121	15.375	17.429	1.00	33.65
60	ATOM	3234	CA	HIS	B	476	14.421	14.886	16.992	1.00	33.31
	ATOM	3235	CB	HIS	B	476	14.782	15.481	15.637	1.00	37.30



5	ATOM	3236	CG	HIS	B	476	14.132	14.781	14.486	1.00	43.64
	ATOM	3237	CD2	HIS	B	476	13.723	13.498	14.342	1.00	45.25
	ATOM	3238	ND1	HIS	B	476	13.816	15.419	13.306	1.00	48.37
	ATOM	3239	CE1	HIS	B	476	13.238	14.560	12.484	1.00	48.87
	ATOM	3240	NE2	HIS	B	476	13.170	13.387	13.089	1.00	48.11
10	ATOM	3241	C	HIS	B	476	15.506	15.213	18.022	1.00	31.20
	ATOM	3242	O	HIS	B	476	16.442	14.436	18.208	1.00	27.25
	ATOM	3243	N	ARG	B	477	15.387	16.365	18.684	1.00	30.64
	ATOM	3244	CA	ARG	B	477	16.361	16.754	19.703	1.00	30.09
	ATOM	3245	CB	ARG	B	477	16.144	18.214	20.121	1.00	33.46
15	ATOM	3246	CG	ARG	B	477	16.322	19.212	18.982	1.00	40.74
	ATOM	3247	CD	ARG	B	477	16.274	20.649	19.479	1.00	45.91
	ATOM	3248	NE	ARG	B	477	17.514	21.020	20.155	1.00	51.37
	ATOM	3249	CZ	ARG	B	477	18.375	21.927	19.702	1.00	53.68
	ATOM	3250	NH1	ARG	B	477	18.140	22.567	18.560	1.00	53.04
20	ATOM	3251	NH2	ARG	B	477	19.480	22.185	20.389	1.00	51.79
	ATOM	3252	C	ARG	B	477	16.232	15.835	20.925	1.00	26.97
	ATOM	3253	O	ARG	B	477	17.233	15.387	21.486	1.00	27.34
	ATOM	3254	N	VAL	B	478	14.999	15.558	21.338	1.00	23.70
	ATOM	3255	CA	VAL	B	478	14.780	14.685	22.482	1.00	24.79
25	ATOM	3256	CB	VAL	B	478	13.286	14.613	22.861	1.00	24.83
	ATOM	3257	CG1	VAL	B	478	13.088	13.646	24.022	1.00	26.23
	ATOM	3258	CG2	VAL	B	478	12.781	15.996	23.243	1.00	28.26
	ATOM	3259	C	VAL	B	478	15.284	13.294	22.112	1.00	26.10
	ATOM	3260	O	VAL	B	478	15.919	12.613	22.927	1.00	24.28
30	ATOM	3261	N	LEU	B	479	15.021	12.889	20.870	1.00	22.92
	ATOM	3262	CA	LEU	B	479	15.456	11.584	20.379	1.00	21.96
	ATOM	3263	CB	LEU	B	479	14.992	11.372	18.930	1.00	22.63
	ATOM	3264	CG	LEU	B	479	13.575	10.798	18.756	1.00	20.82
	ATOM	3265	CD1	LEU	B	479	13.231	10.689	17.274	1.00	22.53
35	ATOM	3266	CD2	LEU	B	479	13.495	9.440	19.420	1.00	23.08
	ATOM	3267	C	LEU	B	479	16.975	11.471	20.453	1.00	21.90
	ATOM	3268	O	LEU	B	479	17.506	10.416	20.778	1.00	23.11
	ATOM	3269	N	ASP	B	480	17.675	12.560	20.143	1.00	23.65
	ATOM	3270	CA	ASP	B	480	19.141	12.566	20.198	1.00	24.29
40	ATOM	3271	CB	ASP	B	480	19.692	13.889	19.649	1.00	26.88
	ATOM	3272	CG	ASP	B	480	19.773	13.914	18.129	1.00	33.32
	ATOM	3273	OD1	ASP	B	480	19.857	12.836	17.499	1.00	35.44
	ATOM	3274	OD2	ASP	B	480	19.757	15.022	17.563	1.00	32.44
	ATOM	3275	C	ASP	B	480	19.590	12.406	21.656	1.00	24.13
45	ATOM	3276	O	ASP	B	480	20.551	11.697	21.956	1.00	24.88
	ATOM	3277	N	LYS	B	481	18.887	13.077	22.560	1.00	25.18
	ATOM	3278	CA	LYS	B	481	19.213	13.010	23.980	1.00	26.78
	ATOM	3279	CB	LYS	B	481	18.262	13.898	24.785	1.00	31.37
	ATOM	3280	CG	LYS	B	481	18.962	14.788	25.804	1.00	43.84
50	ATOM	3281	CD	LYS	B	481	18.780	14.260	27.219	1.00	46.08
	ATOM	3282	CE	LYS	B	481	20.120	13.928	27.865	1.00	50.99
	ATOM	3283	NZ	LYS	B	481	21.177	14.922	27.511	1.00	54.35
	ATOM	3284	C	LYS	B	481	19.124	11.575	24.495	1.00	26.87
	ATOM	3285	O	LYS	B	481	19.951	11.145	25.305	1.00	20.37
55	ATOM	3286	N	ILE	B	482	18.124	10.830	24.027	1.00	23.26
	ATOM	3287	CA	ILE	B	482	17.981	9.452	24.472	1.00	21.07
	ATOM	3288	CB	ILE	B	482	16.655	8.828	24.015	1.00	19.80
	ATOM	3289	CG2	ILE	B	482	16.580	7.370	24.491	1.00	17.40
	ATOM	3290	CG1	ILE	B	482	15.479	9.606	24.602	1.00	17.16
60	ATOM	3291	CD1	ILE	B	482	14.136	9.209	23.991	1.00	19.43
	ATOM	3292	C	ILE	B	482	19.135	8.616	23.947	1.00	20.21

5	ATOM	3293	O	ILE	B	482	19.621	7.722	24.640	1.00	25.55
	ATOM	3294	N	THR	B	483	19.569	8.896	22.722	1.00	21.89
	ATOM	3295	CA	THR	B	483	20.701	8.176	22.141	1.00	22.67
	ATOM	3296	CB	THR	B	483	21.030	8.662	20.695	1.00	23.34
	ATOM	3297	OG1	THR	B	483	19.890	8.475	19.851	1.00	27.33
10	ATOM	3298	CG2	THR	B	483	22.203	7.882	20.116	1.00	24.46
	ATOM	3299	C	THR	B	483	21.913	8.441	23.035	1.00	23.51
	ATOM	3300	O	THR	B	483	22.650	7.520	23.381	1.00	27.01
	ATOM	3301	N	ASP	B	484	22.119	9.703	23.404	1.00	22.88
	ATOM	3302	CA	ASP	B	484	23.237	10.058	24.276	1.00	24.93
15	ATOM	3303	CB	ASP	B	484	23.201	11.546	24.652	1.00	28.69
	ATOM	3304	CG	ASP	B	484	23.504	12.464	23.485	1.00	29.19
	ATOM	3305	OD1	ASP	B	484	23.982	11.984	22.437	1.00	29.63
	ATOM	3306	OD2	ASP	B	484	23.256	13.681	23.627	1.00	32.02
	ATOM	3307	C	ASP	B	484	23.125	9.249	25.567	1.00	24.40
20	ATOM	3308	O	ASP	B	484	24.125	8.780	26.103	1.00	25.60
	ATOM	3309	N	THR	B	485	21.899	9.096	26.066	1.00	20.16
	ATOM	3310	CA	THR	B	485	21.670	8.365	27.307	1.00	22.28
	ATOM	3311	CB	THR	B	485	20.203	8.521	27.763	1.00	24.64
	ATOM	3312	OG1	THR	B	485	19.878	9.914	27.830	1.00	24.28
25	ATOM	3313	CG2	THR	B	485	19.993	7.896	29.133	1.00	23.32
	ATOM	3314	C	THR	B	485	22.017	6.881	27.188	1.00	22.13
	ATOM	3315	O	THR	B	485	22.574	6.284	28.115	1.00	23.30
	ATOM	3316	N	LEU	B	486	21.686	6.290	26.045	1.00	23.08
	ATOM	3317	CA	LEU	B	486	21.969	4.881	25.792	1.00	22.26
30	ATOM	3318	CB	LEU	B	486	21.346	4.452	24.464	1.00	20.93
	ATOM	3319	CG	LEU	B	486	19.878	4.031	24.533	1.00	24.92
	ATOM	3320	CD1	LEU	B	486	19.295	4.003	23.123	1.00	21.96
	ATOM	3321	CD2	LEU	B	486	19.763	2.658	25.196	1.00	23.90
	ATOM	3322	C	LEU	B	486	23.477	4.634	25.742	1.00	24.12
35	ATOM	3323	O	LEU	B	486	23.984	3.681	26.334	1.00	24.02
	ATOM	3324	N	ILE	B	487	24.191	5.490	25.022	1.00	24.53
	ATOM	3325	CA	ILE	B	487	25.640	5.345	24.913	1.00	25.16
	ATOM	3326	CB	ILE	B	487	26.207	6.379	23.899	1.00	25.57
	ATOM	3327	CG2	ILE	B	487	27.725	6.522	24.051	1.00	24.54
40	ATOM	3328	CG1	ILE	B	487	25.857	5.936	22.470	1.00	25.63
	ATOM	3329	CD1	ILE	B	487	26.538	4.646	22.021	1.00	25.68
	ATOM	3330	C	ILE	B	487	26.275	5.518	26.307	1.00	23.60
	ATOM	3331	O	ILE	B	487	27.200	4.794	26.671	1.00	23.65
	ATOM	3332	N	HIS	B	488	25.755	6.456	27.081	1.00	21.75
45	ATOM	3333	CA	HIS	B	488	26.251	6.720	28.431	1.00	26.07
	ATOM	3334	CB	HIS	B	488	25.450	7.871	29.041	1.00	26.99
	ATOM	3335	CG	HIS	B	488	25.818	8.196	30.455	1.00	33.06
	ATOM	3336	CD2	HIS	B	488	25.245	7.838	31.629	1.00	32.79
	ATOM	3337	ND1	HIS	B	488	26.869	9.025	30.779	1.00	36.45
50	ATOM	3338	CE1	HIS	B	488	26.927	9.164	32.091	1.00	35.93
	ATOM	3339	NE2	HIS	B	488	25.953	8.453	32.630	1.00	33.88
	ATOM	3340	C	HIS	B	488	26.123	5.463	29.292	1.00	26.85
	ATOM	3341	O	HIS	B	488	27.071	5.054	29.967	1.00	28.52
	ATOM	3342	N	LEU	B	489	24.949	4.850	29.266	1.00	28.00
55	ATOM	3343	CA	LEU	B	489	24.715	3.642	30.040	1.00	25.94
	ATOM	3344	CB	LEU	B	489	23.298	3.127	29.788	1.00	27.07
	ATOM	3345	CG	LEU	B	489	22.158	3.909	30.445	1.00	31.71
	ATOM	3346	CD1	LEU	B	489	20.827	3.516	29.799	1.00	28.08
	ATOM	3347	CD2	LEU	B	489	22.143	3.616	31.949	1.00	29.30
60	ATOM	3348	C	LEU	B	489	25.718	2.561	29.642	1.00	26.84
	ATOM	3349	O	LEU	B	489	26.241	1.832	30.486	1.00	20.86

5	ATOM	3350	N	MET	B	490	25.978	2.453	28.345	1.00	23.82
	ATOM	3351	CA	MET	B	490	26.900	1.438	27.857	1.00	26.38
	ATOM	3352	CB	MET	B	490	26.775	1.306	26.336	1.00	27.29
	ATOM	3353	CG	MET	B	490	25.418	0.776	25.895	1.00	21.68
	ATOM	3354	SD	MET	B	490	25.208	0.739	24.106	1.00	26.30
10	ATOM	3355	CE	MET	B	490	23.461	0.412	24.022	1.00	19.66
	ATOM	3356	C	MET	B	490	28.341	1.743	28.247	1.00	26.42
	ATOM	3357	O	MET	B	490	29.109	0.833	28.574	1.00	24.76
	ATOM	3358	N	ALA	B	491	28.713	3.018	28.207	1.00	26.67
	ATOM	3359	CA	ALA	B	491	30.074	3.394	28.577	1.00	30.73
15	ATOM	3360	CB	ALA	B	491	30.299	4.882	28.335	1.00	26.66
	ATOM	3361	C	ALA	B	491	30.250	3.053	30.056	1.00	32.08
	ATOM	3362	O	ALA	B	491	31.194	2.361	30.438	1.00	34.66
	ATOM	3363	N	LYS	B	492	29.316	3.523	30.878	1.00	33.17
	ATOM	3364	CA	LYS	B	492	29.354	3.267	32.309	1.00	32.82
20	ATOM	3365	CB	LYS	B	492	28.110	3.849	32.976	1.00	36.38
	ATOM	3366	CG	LYS	B	492	28.412	4.797	34.123	1.00	38.68
	ATOM	3367	CD	LYS	B	492	27.242	4.887	35.084	1.00	41.41
	ATOM	3368	CE	LYS	B	492	26.299	6.013	34.698	1.00	47.57
	ATOM	3369	NZ	LYS	B	492	26.395	7.184	35.618	1.00	50.76
25	ATOM	3370	C	LYS	B	492	29.453	1.771	32.619	1.00	34.08
	ATOM	3371	O	LYS	B	492	30.090	1.382	33.593	1.00	34.31
	ATOM	3372	N	ALA	B	493	28.835	0.935	31.788	1.00	32.03
	ATOM	3373	CA	ALA	B	493	28.867	-0.510	31.998	1.00	30.70
	ATOM	3374	CB	ALA	B	493	27.719	-1.181	31.245	1.00	28.80
30	ATOM	3375	C	ALA	B	493	30.201	-1.156	31.606	1.00	33.75
	ATOM	3376	O	ALA	B	493	30.402	-2.356	31.819	1.00	30.53
	ATOM	3377	N	GLY	B	494	31.102	-0.372	31.020	1.00	33.50
	ATOM	3378	CA	GLY	B	494	32.405	-0.903	30.656	1.00	33.71
	ATOM	3379	C	GLY	B	494	32.639	-1.360	29.230	1.00	34.40
35	ATOM	3380	O	GLY	B	494	33.663	-1.989	28.950	1.00	33.13
	ATOM	3381	N	LEU	B	495	31.712	-1.056	28.326	1.00	31.76
	ATOM	3382	CA	LEU	B	495	31.859	-1.452	26.925	1.00	30.57
	ATOM	3383	CB	LEU	B	495	30.494	-1.415	26.216	1.00	30.67
	ATOM	3384	CG	LEU	B	495	29.610	-2.675	26.256	1.00	29.59
40	ATOM	3385	CD1	LEU	B	495	29.315	-3.058	27.700	1.00	26.60
	ATOM	3386	CD2	LEU	B	495	28.307	-2.416	25.501	1.00	27.52
	ATOM	3387	C	LEU	B	495	32.829	-0.515	26.202	1.00	30.53
	ATOM	3388	O	LEU	B	495	32.855	0.688	26.468	1.00	28.14
	ATOM	3389	N	THR	B	496	33.628	-1.064	25.291	1.00	28.03
45	ATOM	3390	CA	THR	B	496	34.567	-0.243	24.529	1.00	29.06
	ATOM	3391	CB	THR	B	496	35.511	-1.095	23.665	1.00	29.40
	ATOM	3392	OG1	THR	B	496	34.753	-1.758	22.641	1.00	30.29
	ATOM	3393	CG2	THR	B	496	36.228	-2.122	24.515	1.00	28.12
	ATOM	3394	C	THR	B	496	33.770	0.652	23.590	1.00	30.12
50	ATOM	3395	O	THR	B	496	32.580	0.433	23.380	1.00	29.74
	ATOM	3396	N	LEU	B	497	34.430	1.654	23.018	1.00	30.44
	ATOM	3397	CA	LEU	B	497	33.762	2.567	22.104	1.00	28.54
	ATOM	3398	CB	LEU	B	497	34.768	3.564	21.529	1.00	31.14
	ATOM	3399	CG	LEU	B	497	35.209	4.719	22.434	1.00	33.58
55	ATOM	3400	CD1	LEU	B	497	36.120	5.659	21.652	1.00	31.42
	ATOM	3401	CD2	LEU	B	497	33.992	5.469	22.942	1.00	35.08
	ATOM	3402	C	LEU	B	497	33.095	1.800	20.967	1.00	27.35
	ATOM	3403	O	LEU	B	497	31.967	2.105	20.574	1.00	24.03
	ATOM	3404	N	GLN	B	498	33.798	0.797	20.447	1.00	26.17
60	ATOM	3405	CA	GLN	B	498	33.289	-0.009	19.348	1.00	26.32
	ATOM	3406	CB	GLN	B	498	34.411	-0.876	18.771	1.00	27.25

5	ATOM	3407	CG	GLN	B	498	33.967	-1.796	17.645	1.00	32.67
	ATOM	3408	CD	GLN	B	498	34.965	-2.912	17.374	1.00	38.39
	ATOM	3409	OE1	GLN	B	498	35.737	-3.298	18.254	1.00	36.78
	ATOM	3410	NE2	GLN	B	498	34.953	-3.437	16.153	1.00	33.18
	ATOM	3411	C	GLN	B	498	32.112	-0.888	19.774	1.00	25.70
10	ATOM	3412	O	GLN	B	498	31.167	-1.076	19.009	1.00	25.35
	ATOM	3413	N	GLN	B	499	32.173	-1.434	20.986	1.00	24.01
	ATOM	3414	CA	GLN	B	499	31.093	-2.281	21.487	1.00	25.34
	ATOM	3415	CB	GLN	B	499	31.501	-2.935	22.815	1.00	28.38
	ATOM	3416	CG	GLN	B	499	32.537	-4.056	22.669	1.00	29.13
15	ATOM	3417	CD	GLN	B	499	32.913	-4.687	23.995	1.00	30.80
	ATOM	3418	OE1	GLN	B	499	33.306	-3.997	24.937	1.00	33.62
	ATOM	3419	NE2	GLN	B	499	32.797	-6.004	24.074	1.00	30.64
	ATOM	3420	C	GLN	B	499	29.842	-1.430	21.693	1.00	25.70
	ATOM	3421	O	GLN	B	499	28.715	-1.910	21.554	1.00	26.22
20	ATOM	3422	N	GLN	B	500	30.062	-0.160	22.020	1.00	23.09
	ATOM	3423	CA	GLN	B	500	28.989	0.793	22.256	1.00	23.53
	ATOM	3424	CB	GLN	B	500	29.564	2.107	22.782	1.00	26.17
	ATOM	3425	CG	GLN	B	500	29.958	2.073	24.252	1.00	27.71
	ATOM	3426	CD	GLN	B	500	30.812	3.262	24.641	1.00	29.32
25	ATOM	3427	OE1	GLN	B	500	30.559	4.386	24.207	1.00	28.48
	ATOM	3428	NE2	GLN	B	500	31.831	3.021	25.463	1.00	25.07
	ATOM	3429	C	GLN	B	500	28.151	1.074	21.015	1.00	24.24
	ATOM	3430	O	GLN	B	500	26.923	0.949	21.053	1.00	24.40
	ATOM	3431	N	HIS	B	501	28.790	1.465	19.915	1.00	23.08
30	ATOM	3432	CA	HIS	B	501	28.004	1.739	18.724	1.00	26.92
	ATOM	3433	CB	HIS	B	501	28.791	2.577	17.697	1.00	32.00
	ATOM	3434	CG	HIS	B	501	29.988	1.896	17.105	1.00	36.97
	ATOM	3435	CD2	HIS	B	501	30.122	0.710	16.465	1.00	40.32
	ATOM	3436	ND1	HIS	B	501	31.224	2.505	17.042	1.00	37.88
35	ATOM	3437	CE1	HIS	B	501	32.066	1.724	16.389	1.00	38.81
	ATOM	3438	NE2	HIS	B	501	31.422	0.628	16.028	1.00	41.21
	ATOM	3439	C	HIS	B	501	27.451	0.457	18.123	1.00	25.91
	ATOM	3440	O	HIS	B	501	26.369	0.457	17.531	1.00	20.13
	ATOM	3441	N	GLN	B	502	28.165	-0.648	18.317	1.00	24.94
40	ATOM	3442	CA	GLN	B	502	27.698	-1.926	17.804	1.00	21.88
	ATOM	3443	CB	GLN	B	502	28.785	-2.996	17.953	1.00	24.62
	ATOM	3444	CG	GLN	B	502	29.796	-3.001	16.797	1.00	26.55
	ATOM	3445	CD	GLN	B	502	30.843	-4.109	16.902	1.00	27.06
	ATOM	3446	OE1	GLN	B	502	30.716	-5.033	17.705	1.00	28.49
45	ATOM	3447	NE2	GLN	B	502	31.882	-4.018	16.078	1.00	21.90
	ATOM	3448	C	GLN	B	502	26.428	-2.341	18.554	1.00	22.39
	ATOM	3449	O	GLN	B	502	25.464	-2.807	17.944	1.00	22.24
	ATOM	3450	N	ARG	B	503	26.421	-2.159	19.874	1.00	20.54
	ATOM	3451	CA	ARG	B	503	25.259	-2.523	20.678	1.00	22.04
50	ATOM	3452	CB	ARG	B	503	25.602	-2.519	22.180	1.00	22.51
	ATOM	3453	CG	ARG	B	503	24.451	-3.022	23.077	1.00	23.34
	ATOM	3454	CD	ARG	B	503	24.853	-3.110	24.550	1.00	22.18
	ATOM	3455	NE	ARG	B	503	23.743	-3.546	25.395	1.00	19.62
	ATOM	3456	CZ	ARG	B	503	23.329	-4.807	25.497	1.00	19.88
55	ATOM	3457	NH1	ARG	B	503	23.933	-5.765	24.809	1.00	16.40
	ATOM	3458	NH2	ARG	B	503	22.303	-5.110	26.280	1.00	19.71
	ATOM	3459	C	ARG	B	503	24.102	-1.558	20.409	1.00	19.05
	ATOM	3460	O	ARG	B	503	22.945	-1.968	20.351	1.00	18.87
	ATOM	3461	N	LEU	B	504	24.414	-0.276	20.239	1.00	20.19
60	ATOM	3462	CA	LEU	B	504	23.375	0.714	19.969	1.00	19.33
	ATOM	3463	CB	LEU	B	504	23.972	2.117	19.855	1.00	16.25

5	ATOM	3464	CG	LEU	B	504	22.983	3.173	19.344	1.00	20.35
	ATOM	3465	CD1	LEU	B	504	21.930	3.449	20.427	1.00	17.97
	ATOM	3466	CD2	LEU	B	504	23.729	4.448	18.955	1.00	20.86
	ATOM	3467	C	LEU	B	504	22.659	0.357	18.667	1.00	21.22
	ATOM	3468	O	LEU	B	504	21.433	0.478	18.566	1.00	19.28
10	ATOM	3469	N	ALA	B	505	23.428	-0.085	17.676	1.00	18.55
	ATOM	3470	CA	ALA	B	505	22.859	-0.473	16.396	1.00	18.20
	ATOM	3471	CB	ALA	B	505	23.973	-0.745	15.382	1.00	18.45
	ATOM	3472	C	ALA	B	505	21.986	-1.716	16.562	1.00	19.54
	ATOM	3473	O	ALA	B	505	20.871	-1.774	16.041	1.00	17.63
15	ATOM	3474	N	GLN	B	506	22.497	-2.706	17.293	1.00	20.30
	ATOM	3475	CA	GLN	B	506	21.772	-3.955	17.513	1.00	19.48
	ATOM	3476	CB	GLN	B	506	22.590	-4.893	18.409	1.00	21.75
	ATOM	3477	CG	GLN	B	506	23.798	-5.551	17.727	1.00	20.85
	ATOM	3478	CD	GLN	B	506	24.819	-6.070	18.736	1.00	26.18
20	ATOM	3479	OE1	GLN	B	506	24.564	-6.084	19.943	1.00	21.83
	ATOM	3480	NE2	GLN	B	506	25.977	-6.499	18.245	1.00	25.39
	ATOM	3481	C	GLN	B	506	20.421	-3.672	18.166	1.00	21.39
	ATOM	3482	O	GLN	B	506	19.396	-4.233	17.766	1.00	20.87
	ATOM	3483	N	LEU	B	507	20.433	-2.800	19.171	1.00	19.52
25	ATOM	3484	CA	LEU	B	507	19.219	-2.418	19.884	1.00	23.04
	ATOM	3485	CB	LEU	B	507	19.548	-1.455	21.030	1.00	22.82
	ATOM	3486	CG	LEU	B	507	20.182	-2.011	22.313	1.00	26.12
	ATOM	3487	CD1	LEU	B	507	20.203	-0.916	23.360	1.00	29.33
	ATOM	3488	CD2	LEU	B	507	19.415	-3.213	22.816	1.00	27.80
30	ATOM	3489	C	LEU	B	507	18.212	-1.730	18.971	1.00	22.19
	ATOM	3490	O	LEU	B	507	17.036	-2.070	18.964	1.00	23.00
	ATOM	3491	N	LEU	B	508	18.678	-0.745	18.214	1.00	21.53
	ATOM	3492	CA	LEU	B	508	17.797	0.006	17.332	1.00	20.60
	ATOM	3493	CB	LEU	B	508	18.535	1.236	16.805	1.00	17.57
35	ATOM	3494	CG	LEU	B	508	18.934	2.218	17.913	1.00	17.67
	ATOM	3495	CD1	LEU	B	508	19.566	3.446	17.301	1.00	20.04
	ATOM	3496	CD2	LEU	B	508	17.724	2.611	18.725	1.00	18.49
	ATOM	3497	C	LEU	B	508	17.235	-0.831	16.183	1.00	21.17
	ATOM	3498	O	LEU	B	508	16.118	-0.597	15.728	1.00	21.88
40	ATOM	3499	N	LEU	B	509	18.000	-1.813	15.713	1.00	21.89
	ATOM	3500	CA	LEU	B	509	17.511	-2.657	14.631	1.00	22.81
	ATOM	3501	CB	LEU	B	509	18.603	-3.597	14.145	1.00	22.65
	ATOM	3502	CG	LEU	B	509	19.645	-2.891	13.278	1.00	29.11
	ATOM	3503	CD1	LEU	B	509	20.697	-3.888	12.829	1.00	25.69
45	ATOM	3504	CD2	LEU	B	509	18.965	-2.248	12.082	1.00	27.92
	ATOM	3505	C	LEU	B	509	16.302	-3.462	15.095	1.00	23.32
	ATOM	3506	O	LEU	B	509	15.409	-3.759	14.303	1.00	23.36
	ATOM	3507	N	ILE	B	510	16.264	-3.796	16.380	1.00	23.36
	ATOM	3508	CA	ILE	B	510	15.148	-4.562	16.912	1.00	20.99
50	ATOM	3509	CB	ILE	B	510	15.448	-5.041	18.361	1.00	28.60
	ATOM	3510	CG2	ILE	B	510	14.162	-5.435	19.075	1.00	28.10
	ATOM	3511	CG1	ILE	B	510	16.383	-6.260	18.308	1.00	26.57
	ATOM	3512	CD1	ILE	B	510	17.429	-6.301	19.419	1.00	30.14
	ATOM	3513	C	ILE	B	510	13.852	-3.746	16.846	1.00	17.65
55	ATOM	3514	O	ILE	B	510	12.767	-4.308	16.759	1.00	16.11
	ATOM	3515	N	LEU	B	511	13.961	-2.421	16.867	1.00	18.12
	ATOM	3516	CA	LEU	B	511	12.772	-1.574	16.774	1.00	16.95
	ATOM	3517	CB	LEU	B	511	13.147	-0.100	16.981	1.00	22.66
	ATOM	3518	CG	LEU	B	511	13.607	0.262	18.406	1.00	22.13
60	ATOM	3519	CD1	LEU	B	511	13.404	1.751	18.652	1.00	25.29
	ATOM	3520	CD2	LEU	B	511	12.830	-0.549	19.425	1.00	25.08

5	ATOM	3521	C	LEU	B	511	12.112	-1.771	15.397	1.00	16.65
	ATOM	3522	O	LEU	B	511	10.915	-1.578	15.242	1.00	17.09
	ATOM	3523	N	SER	B	512	12.901	-2.161	14.401	1.00	15.83
	ATOM	3524	CA	SER	B	512	12.355	-2.408	13.072	1.00	18.66
	ATOM	3525	CB	SER	B	512	13.484	-2.644	12.074	1.00	17.62
10	ATOM	3526	OG	SER	B	512	13.079	-3.550	11.062	1.00	32.77
	ATOM	3527	C	SER	B	512	11.454	-3.638	13.154	1.00	18.54
	ATOM	3528	O	SER	B	512	10.373	-3.683	12.545	1.00	17.01
	ATOM	3529	N	HIS	B	513	11.899	-4.625	13.929	1.00	15.54
	ATOM	3530	CA	HIS	B	513	11.141	-5.860	14.115	1.00	17.67
15	ATOM	3531	CB	HIS	B	513	12.013	-6.916	14.790	1.00	19.03
	ATOM	3532	CG	HIS	B	513	13.063	-7.475	13.886	1.00	27.06
	ATOM	3533	CD2	HIS	B	513	12.980	-8.364	12.868	1.00	28.40
	ATOM	3534	ND1	HIS	B	513	14.378	-7.066	13.932	1.00	28.92
	ATOM	3535	CE1	HIS	B	513	15.061	-7.678	12.981	1.00	30.75
20	ATOM	3536	NE2	HIS	B	513	14.235	-8.472	12.321	1.00	30.08
	ATOM	3537	C	HIS	B	513	9.895	-5.602	14.958	1.00	15.35
	ATOM	3538	O	HIS	B	513	8.846	-6.192	14.704	1.00	14.83
	ATOM	3539	N	ILE	B	514	10.012	-4.744	15.942	1.00	13.35
	ATOM	3540	CA	ILE	B	514	8.865	-4.417	16.776	1.00	15.48
25	ATOM	3541	CB	ILE	B	514	9.295	-3.534	17.967	1.00	20.02
	ATOM	3542	CG2	ILE	B	514	8.067	-2.918	18.650	1.00	12.84
	ATOM	3543	CG1	ILE	B	514	10.093	-4.397	18.962	1.00	22.87
	ATOM	3544	CD1	ILE	B	514	10.691	-3.641	20.115	1.00	29.62
	ATOM	3545	C	ILE	B	514	7.797	-3.717	15.923	1.00	15.16
30	ATOM	3546	O	ILE	B	514	6.606	-3.972	16.078	1.00	16.61
	ATOM	3547	N	ARG	B	515	8.224	-2.823	15.030	1.00	16.33
	ATOM	3548	CA	ARG	B	515	7.280	-2.138	14.150	1.00	17.54
	ATOM	3549	CB	ARG	B	515	8.010	-1.173	13.214	1.00	20.15
	ATOM	3550	CG	ARG	B	515	7.080	-0.454	12.234	1.00	21.47
35	ATOM	3551	CD	ARG	B	515	6.407	0.749	12.891	1.00	26.05
	ATOM	3552	NE	ARG	B	515	7.220	1.948	12.716	1.00	24.91
	ATOM	3553	CZ	ARG	B	515	6.734	3.175	12.547	1.00	24.61
	ATOM	3554	NH1	ARG	B	515	5.424	3.393	12.522	1.00	22.46
	ATOM	3555	NH2	ARG	B	515	7.569	4.182	12.374	1.00	23.15
40	ATOM	3556	C	ARG	B	515	6.545	-3.182	13.304	1.00	16.60
	ATOM	3557	O	ARG	B	515	5.332	-3.093	13.087	1.00	14.51
	ATOM	3558	N	HIS	B	516	7.298	-4.171	12.827	1.00	18.50
	ATOM	3559	CA	HIS	B	516	6.743	-5.237	11.997	1.00	17.26
	ATOM	3560	CB	HIS	B	516	7.861	-6.176	11.533	1.00	18.14
45	ATOM	3561	CG	HIS	B	516	7.405	-7.223	10.568	1.00	24.87
	ATOM	3562	CD2	HIS	B	516	7.060	-8.521	10.754	1.00	26.64
	ATOM	3563	ND1	HIS	B	516	7.258	-6.978	9.220	1.00	21.82
	ATOM	3564	CE1	HIS	B	516	6.839	-8.078	8.619	1.00	28.42
	ATOM	3565	NE2	HIS	B	516	6.711	-9.028	9.526	1.00	24.47
50	ATOM	3566	C	HIS	B	516	5.685	-6.028	12.759	1.00	16.87
	ATOM	3567	O	HIS	B	516	4.596	-6.303	12.240	1.00	14.81
	ATOM	3568	N	MET	B	517	5.999	-6.396	13.997	1.00	16.48
	ATOM	3569	CA	MET	B	517	5.049	-7.162	14.801	1.00	15.39
	ATOM	3570	CB	MET	B	517	5.701	-7.587	16.114	1.00	21.05
55	ATOM	3571	CG	MET	B	517	6.790	-8.638	15.917	1.00	20.76
	ATOM	3572	SD	MET	B	517	7.380	-9.320	17.470	1.00	23.96
	ATOM	3573	CE	MET	B	517	8.104	-7.879	18.226	1.00	20.45
	ATOM	3574	C	MET	B	517	3.789	-6.368	15.080	1.00	16.23
	ATOM	3575	O	MET	B	517	2.688	-6.924	15.148	1.00	16.02
60	ATOM	3576	N	SER	B	518	3.954	-5.060	15.247	1.00	13.32
	ATOM	3577	CA	SER	B	518	2.827	-4.186	15.505	1.00	16.34

5	ATOM	3578	CB	SER	B	518	3.316	-2.765	15.835	1.00	17.48
	ATOM	3579	OG	SER	B	518	2.234	-1.840	15.843	1.00	17.46
	ATOM	3580	C	SER	B	518	1.906	-4.147	14.284	1.00	14.73
	ATOM	3581	O	SER	B	518	0.688	-4.247	14.417	1.00	19.16
	ATOM	3582	N	ASN	B	519	2.474	-4.006	13.091	1.00	14.52
10	ATOM	3583	CA	ASN	B	519	1.622	-3.953	11.907	1.00	15.35
	ATOM	3584	CB	ASN	B	519	2.432	-3.509	10.698	1.00	19.21
	ATOM	3585	CG	ASN	B	519	2.700	-2.029	10.729	1.00	20.58
	ATOM	3586	OD1	ASN	B	519	1.839	-1.258	11.150	1.00	26.36
	ATOM	3587	ND2	ASN	B	519	3.891	-1.618	10.307	1.00	19.62
15	ATOM	3588	C	ASN	B	519	0.911	-5.280	11.658	1.00	16.74
	ATOM	3589	O	ASN	B	519	-0.265	-5.299	11.297	1.00	20.58
	ATOM	3590	N	LYS	B	520	1.608	-6.387	11.885	1.00	18.60
	ATOM	3591	CA	LYS	B	520	0.992	-7.699	11.717	1.00	20.04
	ATOM	3592	CB	LYS	B	520	2.038	-8.801	11.872	1.00	25.44
20	ATOM	3593	CG	LYS	B	520	3.037	-8.849	10.728	1.00	31.68
	ATOM	3594	CD	LYS	B	520	2.507	-9.663	9.558	1.00	42.56
	ATOM	3595	CE	LYS	B	520	2.186	-8.778	8.364	1.00	45.61
	ATOM	3596	NZ	LYS	B	520	1.435	-9.526	7.312	1.00	46.00
	ATOM	3597	C	LYS	B	520	-0.099	-7.868	12.769	1.00	18.88
25	ATOM	3598	O	LYS	B	520	-1.183	-8.358	12.478	1.00	21.75
	ATOM	3599	N	GLY	B	521	0.191	-7.455	13.998	1.00	17.83
	ATOM	3600	CA	GLY	B	521	-0.792	-7.569	15.058	1.00	16.19
	ATOM	3601	C	GLY	B	521	-2.000	-6.674	14.833	1.00	16.59
	ATOM	3602	O	GLY	B	521	-3.128	-7.060	15.125	1.00	16.57
30	ATOM	3603	N	MET	B	522	-1.766	-5.467	14.326	1.00	17.48
	ATOM	3604	CA	MET	B	522	-2.852	-4.527	14.042	1.00	18.25
	ATOM	3605	CB	MET	B	522	-2.276	-3.212	13.516	1.00	21.27
	ATOM	3606	CG	MET	B	522	-3.190	-2.018	13.707	1.00	26.97
	ATOM	3607	SD	MET	B	522	-3.199	-1.477	15.417	1.00	30.35
35	ATOM	3608	CE	MET	B	522	-1.659	-0.605	15.475	1.00	29.86
	ATOM	3609	C	MET	B	522	-3.794	-5.119	12.989	1.00	18.68
	ATOM	3610	O	MET	B	522	-5.022	-5.008	13.097	1.00	18.80
	ATOM	3611	N	GLU	B	523	-3.205	-5.731	11.966	1.00	18.22
	ATOM	3612	CA	GLU	B	523	-3.968	-6.357	10.889	1.00	23.41
40	ATOM	3613	CB	GLU	B	523	-3.031	-6.946	9.830	1.00	28.74
	ATOM	3614	CG	GLU	B	523	-2.224	-5.935	9.030	1.00	34.42
	ATOM	3615	CD	GLU	B	523	-1.095	-6.597	8.239	1.00	45.58
	ATOM	3616	OE1	GLU	B	523	-0.131	-5.894	7.857	1.00	49.48
	ATOM	3617	OE2	GLU	B	523	-1.169	-7.825	7.999	1.00	45.97
45	ATOM	3618	C	GLU	B	523	-4.812	-7.482	11.465	1.00	23.98
	ATOM	3619	O	GLU	B	523	-5.993	-7.616	11.147	1.00	22.08
	ATOM	3620	N	HIS	B	524	-4.187	-8.287	12.326	1.00	23.46
	ATOM	3621	CA	HIS	B	524	-4.846	-9.428	12.952	1.00	26.20
	ATOM	3622	CB	HIS	B	524	-3.824	-10.245	13.743	1.00	27.26
50	ATOM	3623	CG	HIS	B	524	-4.378	-11.509	14.321	1.00	30.91
	ATOM	3624	CD2	HIS	B	524	-4.308	-12.792	13.892	1.00	30.90
	ATOM	3625	ND1	HIS	B	524	-5.107	-11.537	15.490	1.00	28.87
	ATOM	3626	CE1	HIS	B	524	-5.461	-12.780	15.757	1.00	30.45
	ATOM	3627	NE2	HIS	B	524	-4.989	-13.561	14.803	1.00	29.19
55	ATOM	3628	C	HIS	B	524	-5.996	-9.025	13.870	1.00	27.69
	ATOM	3629	O	HIS	B	524	-7.061	-9.656	13.860	1.00	25.00
	ATOM	3630	N	LEU	B	525	-5.777	-7.977	14.655	1.00	23.84
	ATOM	3631	CA	LEU	B	525	-6.786	-7.492	15.588	1.00	25.77
	ATOM	3632	CB	LEU	B	525	-6.217	-6.358	16.444	1.00	22.22
60	ATOM	3633	CG	LEU	B	525	-7.164	-5.778	17.498	1.00	26.81
	ATOM	3634	CD1	LEU	B	525	-7.763	-6.922	18.321	1.00	23.32

5	ATOM	3635	CD2	LEU	B	525	-6.414	-4.793	18.399	1.00	18.95
	ATOM	3636	C	LEU	B	525	-8.013	-6.995	14.842	1.00	26.84
	ATOM	3637	O	LEU	B	525	-9.154	-7.247	15.249	1.00	26.73
	ATOM	3638	N	TYR	B	526	-7.764	-6.271	13.757	1.00	26.86
	ATOM	3639	CA	TYR	B	526	-8.819	-5.726	12.918	1.00	30.89
10	ATOM	3640	CB	TYR	B	526	-8.201	-4.818	11.854	1.00	34.31
	ATOM	3641	CG	TYR	B	526	-9.183	-4.223	10.878	1.00	43.50
	ATOM	3642	CD1	TYR	B	526	-10.058	-3.211	11.267	1.00	47.66
	ATOM	3643	CE1	TYR	B	526	-10.943	-2.636	10.357	1.00	48.85
	ATOM	3644	CD2	TYR	B	526	-9.218	-4.651	9.552	1.00	48.52
15	ATOM	3645	CE2	TYR	B	526	-10.098	-4.083	8.634	1.00	52.43
	ATOM	3646	CZ	TYR	B	526	-10.955	-3.077	9.043	1.00	51.67
	ATOM	3647	OH	TYR	B	526	-11.810	-2.504	8.129	1.00	57.01
	ATOM	3648	C	TYR	B	526	-9.577	-6.880	12.265	1.00	30.90
	ATOM	3649	O	TYR	B	526	-10.793	-6.829	12.113	1.00	31.48
20	ATOM	3650	N	SER	B	527	-8.849	-7.926	11.889	1.00	31.39
	ATOM	3651	CA	SER	B	527	-9.460	-9.095	11.266	1.00	33.73
	ATOM	3652	CB	SER	B	527	-8.377	-10.048	10.749	1.00	34.13
	ATOM	3653	OG	SER	B	527	-8.945	-11.222	10.196	1.00	43.67
	ATOM	3654	C	SER	B	527	-10.339	-9.813	12.288	1.00	34.34
25	ATOM	3655	O	SER	B	527	-11.446	-10.261	11.973	1.00	33.42
	ATOM	3656	N	MET	B	528	-9.840	-9.916	13.517	1.00	31.66
	ATOM	3657	CA	MET	B	528	-10.574	-10.572	14.589	1.00	29.77
	ATOM	3658	CB	MET	B	528	-9.682	-10.743	15.820	1.00	32.96
	ATOM	3659	CG	MET	B	528	-8.651	-11.859	15.699	1.00	33.47
30	ATOM	3660	SD	MET	B	528	-9.359	-13.427	15.134	1.00	38.28
	ATOM	3661	CE	MET	B	528	-10.265	-13.915	16.579	1.00	36.01
	ATOM	3662	C	MET	B	528	-11.800	-9.747	14.953	1.00	29.42
	ATOM	3663	O	MET	B	528	-12.835	-10.293	15.331	1.00	28.65
	ATOM	3664	N	LYS	B	529	-11.673	-8.429	14.850	1.00	30.64
35	ATOM	3665	CA	LYS	B	529	-12.781	-7.533	15.149	1.00	31.80
	ATOM	3666	CB	LYS	B	529	-12.323	-6.079	15.027	1.00	32.86
	ATOM	3667	CG	LYS	B	529	-13.436	-5.043	15.114	1.00	36.42
	ATOM	3668	CD	LYS	B	529	-13.114	-3.852	14.224	1.00	41.74
	ATOM	3669	CE	LYS	B	529	-13.734	-2.564	14.741	1.00	43.45
40	ATOM	3670	NZ	LYS	B	529	-15.221	-2.569	14.634	1.00	46.51
	ATOM	3671	C	LYS	B	529	-13.857	-7.840	14.116	1.00	36.60
	ATOM	3672	O	LYS	B	529	-15.049	-7.877	14.424	1.00	34.04
	ATOM	3673	N	CYS	B	530	-13.407	-8.083	12.889	1.00	40.04
	ATOM	3674	CA	CYS	B	530	-14.286	-8.409	11.773	1.00	44.58
45	ATOM	3675	CB	CYS	B	530	-13.460	-8.535	10.491	1.00	50.64
	ATOM	3676	SG	CYS	B	530	-13.369	-7.034	9.504	1.00	67.65
	ATOM	3677	C	CYS	B	530	-15.065	-9.692	12.016	1.00	42.88
	ATOM	3678	O	CYS	B	530	-16.274	-9.741	11.807	1.00	40.15
	ATOM	3679	N	LYS	B	531	-14.360	-10.733	12.447	1.00	41.92
50	ATOM	3680	CA	LYS	B	531	-14.980	-12.023	12.728	1.00	42.60
	ATOM	3681	CB	LYS	B	531	-13.907	-13.091	12.927	1.00	44.77
	ATOM	3682	C	LYS	B	531	-15.844	-11.907	13.977	1.00	44.43
	ATOM	3683	O	LYS	B	531	-16.623	-12.804	14.296	1.00	44.09
	ATOM	3684	N	ASN	B	532	-15.678	-10.793	14.685	1.00	44.98
55	ATOM	3685	CA	ASN	B	532	-16.437	-10.496	15.893	1.00	44.10
	ATOM	3686	CB	ASN	B	532	-17.833	-10.003	15.506	1.00	45.14
	ATOM	3687	CG	ASN	B	532	-18.526	-9.271	16.633	1.00	46.54
	ATOM	3688	OD1	ASN	B	532	-19.729	-9.424	16.837	1.00	50.62
	ATOM	3689	ND2	ASN	B	532	-17.771	-8.471	17.375	1.00	46.07
60	ATOM	3690	C	ASN	B	532	-16.557	-11.657	16.882	1.00	43.34
	ATOM	3691	O	ASN	B	532	-17.655	-11.994	17.321	1.00	41.42



5	ATOM	3692	N	VAL	B	533	-15.434	-12.264	17.243	1.00	43.45
	ATOM	3693	CA	VAL	B	533	-15.471	-13.371	18.190	1.00	44.06
	ATOM	3694	CB	VAL	B	533	-14.170	-14.219	18.120	1.00	45.56
	ATOM	3695	CG1	VAL	B	533	-13.661	-14.263	16.683	1.00	45.67
	ATOM	3696	CG2	VAL	B	533	-13.107	-13.644	19.045	1.00	44.16
10	ATOM	3697	C	VAL	B	533	-15.670	-12.835	19.611	1.00	43.24
	ATOM	3698	O	VAL	B	533	-15.894	-13.602	20.548	1.00	44.21
	ATOM	3699	N	VAL	B	534	-15.596	-11.511	19.755	1.00	40.44
	ATOM	3700	CA	VAL	B	534	-15.765	-10.849	21.049	1.00	37.80
	ATOM	3701	CB	VAL	B	534	-14.630	-11.259	22.038	1.00	36.38
15	ATOM	3702	CG1	VAL	B	534	-13.324	-10.575	21.658	1.00	34.35
	ATOM	3703	CG2	VAL	B	534	-15.021	-10.910	23.463	1.00	39.34
	ATOM	3704	C	VAL	B	534	-15.752	-9.329	20.857	1.00	37.97
	ATOM	3705	O	VAL	B	534	-15.026	-8.808	20.008	1.00	39.45
	ATOM	3706	N	PRO	B	535	-16.575	-8.597	21.625	1.00	37.81
20	ATOM	3707	CD	PRO	B	535	-17.529	-9.078	22.640	1.00	38.74
	ATOM	3708	CA	PRO	B	535	-16.608	-7.135	21.492	1.00	36.79
	ATOM	3709	CB	PRO	B	535	-17.846	-6.729	22.288	1.00	36.98
	ATOM	3710	CG	PRO	B	535	-18.004	-7.809	23.298	1.00	39.77
	ATOM	3711	C	PRO	B	535	-15.338	-6.494	22.049	1.00	33.95
25	ATOM	3712	O	PRO	B	535	-14.786	-6.963	23.040	1.00	34.93
	ATOM	3713	N	LEU	B	536	-14.881	-5.426	21.409	1.00	33.42
	ATOM	3714	CA	LEU	B	536	-13.675	-4.732	21.851	1.00	33.40
	ATOM	3715	CB	LEU	B	536	-12.829	-4.314	20.647	1.00	29.31
	ATOM	3716	CG	LEU	B	536	-12.219	-5.433	19.798	1.00	30.06
30	ATOM	3717	CD1	LEU	B	536	-11.344	-4.822	18.714	1.00	30.85
	ATOM	3718	CD2	LEU	B	536	-11.398	-6.370	20.676	1.00	28.96
	ATOM	3719	C	LEU	B	536	-14.036	-3.498	22.666	1.00	30.50
	ATOM	3720	O	LEU	B	536	-15.024	-2.829	22.383	1.00	29.91
	ATOM	3721	N	TYR	B	537	-13.231	-3.194	23.676	1.00	28.69
35	ATOM	3722	CA	TYR	B	537	-13.494	-2.032	24.505	1.00	29.89
	ATOM	3723	CB	TYR	B	537	-12.618	-2.071	25.750	1.00	32.50
	ATOM	3724	CG	TYR	B	537	-12.849	-3.327	26.543	1.00	39.46
	ATOM	3725	CD1	TYR	B	537	-13.923	-3.431	27.421	1.00	41.90
	ATOM	3726	CE1	TYR	B	537	-14.174	-4.609	28.118	1.00	45.72
40	ATOM	3727	CD2	TYR	B	537	-12.022	-4.435	26.379	1.00	47.39
	ATOM	3728	CE2	TYR	B	537	-12.262	-5.620	27.072	1.00	49.93
	ATOM	3729	CZ	TYR	B	537	-13.340	-5.699	27.940	1.00	48.80
	ATOM	3730	OH	TYR	B	537	-13.582	-6.872	28.624	1.00	53.90
	ATOM	3731	C	TYR	B	537	-13.262	-0.761	23.709	1.00	27.09
45	ATOM	3732	O	TYR	B	537	-12.518	-0.757	22.729	1.00	26.15
	ATOM	3733	N	ASP	B	538	-13.909	0.315	24.141	1.00	26.12
	ATOM	3734	CA	ASP	B	538	-13.830	1.598	23.461	1.00	25.27
	ATOM	3735	CB	ASP	B	538	-14.748	2.598	24.164	1.00	28.85
	ATOM	3736	CG	ASP	B	538	-16.227	2.285	23.940	1.00	33.90
50	ATOM	3737	OD1	ASP	B	538	-17.052	2.613	24.819	1.00	32.68
	ATOM	3738	OD2	ASP	B	538	-16.562	1.707	22.882	1.00	38.26
	ATOM	3739	C	ASP	B	538	-12.447	2.217	23.261	1.00	25.18
	ATOM	3740	O	ASP	B	538	-12.120	2.626	22.147	1.00	26.41
	ATOM	3741	N	LEU	B	539	-11.637	2.309	24.313	1.00	20.76
55	ATOM	3742	CA	LEU	B	539	-10.312	2.911	24.150	1.00	19.65
	ATOM	3743	CB	LEU	B	539	-9.567	2.991	25.496	1.00	17.48
	ATOM	3744	CG	LEU	B	539	-8.116	3.511	25.469	1.00	16.46
	ATOM	3745	CD1	LEU	B	539	-8.051	4.892	24.838	1.00	16.43
	ATOM	3746	CD2	LEU	B	539	-7.564	3.569	26.895	1.00	15.57
60	ATOM	3747	C	LEU	B	539	-9.484	2.127	23.127	1.00	16.75
	ATOM	3748	O	LEU	B	539	-8.862	2.716	22.249	1.00	20.36

5	ATOM	3749	N	LEU	B	540	-9.487	0.803	23.239	1.00	18.23
	ATOM	3750	CA	LEU	B	540	-8.743	-0.048	22.319	1.00	18.05
	ATOM	3751	CB	LEU	B	540	-8.909	-1.528	22.701	1.00	16.38
	ATOM	3752	CG	LEU	B	540	-8.188	-2.554	21.821	1.00	19.81
	ATOM	3753	CD1	LEU	B	540	-6.679	-2.303	21.828	1.00	19.27
10	ATOM	3754	CD2	LEU	B	540	-8.473	-3.952	22.327	1.00	18.00
	ATOM	3755	C	LEU	B	540	-9.241	0.169	20.891	1.00	21.50
	ATOM	3756	O	LEU	B	540	-8.449	0.293	19.964	1.00	20.41
	ATOM	3757	N	LEU	B	541	-10.559	0.206	20.726	1.00	22.40
	ATOM	3758	CA	LEU	B	541	-11.164	0.419	19.413	1.00	23.27
15	ATOM	3759	CB	LEU	B	541	-12.686	0.429	19.527	1.00	25.12
	ATOM	3760	CG	LEU	B	541	-13.410	-0.808	18.999	1.00	36.53
	ATOM	3761	CD1	LEU	B	541	-14.910	-0.671	19.273	1.00	30.98
	ATOM	3762	CD2	LEU	B	541	-13.136	-0.971	17.508	1.00	31.93
	ATOM	3763	C	LEU	B	541	-10.697	1.751	18.842	1.00	22.46
20	ATOM	3764	O	LEU	B	541	-10.359	1.845	17.666	1.00	26.29
	ATOM	3765	N	GLU	B	542	-10.694	2.781	19.680	1.00	23.96
	ATOM	3766	CA	GLU	B	542	-10.248	4.106	19.270	1.00	26.91
	ATOM	3767	CB	GLU	B	542	-10.250	5.050	20.468	1.00	30.84
	ATOM	3768	CG	GLU	B	542	-11.166	6.245	20.347	1.00	37.20
25	ATOM	3769	CD	GLU	B	542	-11.138	7.105	21.597	1.00	39.98
	ATOM	3770	OE1	GLU	B	542	-12.223	7.385	22.144	1.00	39.92
	ATOM	3771	OE2	GLU	B	542	-10.028	7.494	22.034	1.00	38.96
	ATOM	3772	C	GLU	B	542	-8.826	4.010	18.724	1.00	27.90
	ATOM	3773	O	GLU	B	542	-8.530	4.492	17.634	1.00	29.32
30	ATOM	3774	N	MET	B	543	-7.945	3.388	19.499	1.00	26.41
	ATOM	3775	CA	MET	B	543	-6.552	3.237	19.107	1.00	23.53
	ATOM	3776	CB	MET	B	543	-5.749	2.591	20.247	1.00	24.60
	ATOM	3777	CG	MET	B	543	-5.812	3.338	21.579	1.00	26.46
	ATOM	3778	SD	MET	B	543	-5.373	5.084	21.467	1.00	29.45
35	ATOM	3779	CE	MET	B	543	-3.585	4.971	21.349	1.00	25.43
	ATOM	3780	C	MET	B	543	-6.403	2.407	17.832	1.00	25.80
	ATOM	3781	O	MET	B	543	-5.535	2.686	17.004	1.00	23.59
	ATOM	3782	N	LEU	B	544	-7.254	1.394	17.673	1.00	27.74
	ATOM	3783	CA	LEU	B	544	-7.202	0.522	16.499	1.00	26.32
40	ATOM	3784	CB	LEU	B	544	-8.069	-0.721	16.719	1.00	26.75
	ATOM	3785	CG	LEU	B	544	-8.274	-1.632	15.502	1.00	28.12
	ATOM	3786	CD1	LEU	B	544	-6.956	-2.294	15.136	1.00	26.36
	ATOM	3787	CD2	LEU	B	544	-9.330	-2.680	15.803	1.00	27.00
	ATOM	3788	C	LEU	B	544	-7.672	1.252	15.250	1.00	26.97
45	ATOM	3789	O	LEU	B	544	-7.036	1.181	14.195	1.00	24.25
	ATOM	3790	N	ASP	B	545	-8.787	1.961	15.372	1.00	30.37
	ATOM	3791	CA	ASP	B	545	-9.338	2.702	14.244	1.00	32.34
	ATOM	3792	CB	ASP	B	545	-10.668	3.346	14.637	1.00	36.61
	ATOM	3793	CG	ASP	B	545	-11.818	2.370	14.565	1.00	42.73
50	ATOM	3794	OD1	ASP	B	545	-12.858	2.624	15.211	1.00	47.39
	ATOM	3795	OD2	ASP	B	545	-11.676	1.342	13.863	1.00	46.96
	ATOM	3796	C	ASP	B	545	-8.382	3.762	13.711	1.00	31.27
	ATOM	3797	O	ASP	B	545	-8.443	4.120	12.532	1.00	30.53
	ATOM	3798	N	ALA	B	546	-7.506	4.272	14.572	1.00	29.02
55	ATOM	3799	CA	ALA	B	546	-6.543	5.280	14.141	1.00	31.21
	ATOM	3800	CB	ALA	B	546	-5.646	5.693	15.306	1.00	30.98
	ATOM	3801	C	ALA	B	546	-5.697	4.731	12.996	1.00	32.14
	ATOM	3802	O	ALA	B	546	-5.189	5.490	12.170	1.00	33.78
	ATOM	3803	N	HIS	B	547	-5.555	3.410	12.943	1.00	32.27
60	ATOM	3804	CA	HIS	B	547	-4.773	2.767	11.892	1.00	37.73
	ATOM	3805	CB	HIS	B	547	-3.991	1.576	12.457	1.00	35.83

5	ATOM	3806	CG	HIS	B	547	-2.796	1.968	13.269	1.00	34.54
	ATOM	3807	CD2	HIS	B	547	-2.698	2.553	14.486	1.00	30.23
	ATOM	3808	ND1	HIS	B	547	-1.502	1.755	12.840	1.00	34.23
	ATOM	3809	CE1	HIS	B	547	-0.659	2.193	13.760	1.00	36.72
	ATOM	3810	NE2	HIS	B	547	-1.360	2.681	14.768	1.00	31.48
10	ATOM	3811	C	HIS	B	547	-5.649	2.286	10.735	1.00	43.69
	ATOM	3812	O	HIS	B	547	-5.178	2.152	9.606	1.00	46.04
	ATOM	3813	N	ARG	B	548	-6.919	2.020	11.019	1.00	48.35
	ATOM	3814	CA	ARG	B	548	-7.843	1.551	9.993	1.00	54.74
	ATOM	3815	CB	ARG	B	548	-8.522	0.267	10.452	1.00	54.66
15	ATOM	3816	C	ARG	B	548	-8.886	2.619	9.681	1.00	59.94
	ATOM	3817	O	ARG	B	548	-8.580	3.812	9.672	1.00	62.81
	ATOM	3818	N	LEU	B	549	-10.116	2.186	9.422	1.00	64.81
	ATOM	3819	CA	LEU	B	549	-11.204	3.109	9.112	1.00	67.59
	ATOM	3820	CB	LEU	B	549	-12.478	2.327	8.799	1.00	68.06
20	ATOM	3821	C	LEU	B	549	-11.449	4.069	10.275	1.00	69.12
	ATOM	3822	O	LEU	B	549	-11.451	5.297	10.036	1.00	68.96
	ATOM	3823	OXT	LEU	B	549	-11.634	3.579	11.412	1.00	70.70
	HETATM	3824	CP9	DES	B	600	-4.547	-6.077	22.000	1.00	18.55
	HETATM	3825	CP8	DES	B	600	-3.163	-6.365	21.467	1.00	17.72
25	HETATM	3826	CP7	DES	B	600	-2.897	-7.853	21.381	1.00	21.17
	HETATM	3827	CP6	DES	B	600	-3.719	-8.551	20.374	1.00	22.05
	HETATM	3828	CP1	DES	B	600	-3.405	-8.481	18.998	1.00	21.32
	HETATM	3829	CP2	DES	B	600	-4.239	-9.095	18.063	1.00	21.61
	HETATM	3830	CP3	DES	B	600	-5.388	-9.771	18.509	1.00	24.89
30	HETATM	3831	OP3	DES	B	600	-6.244	-10.339	17.600	1.00	24.94
	HETATM	3832	CP4	DES	B	600	-5.718	-9.858	19.860	1.00	24.08
	HETATM	3833	CP5	DES	B	600	-4.877	-9.240	20.791	1.00	24.67
	HETATM	3834	C7	DES	B	600	-1.998	-8.460	22.190	1.00	16.67
	HETATM	3835	C6	DES	B	600	-1.330	-7.834	23.325	1.00	15.39
35	HETATM	3836	C5	DES	B	600	-2.054	-7.642	24.522	1.00	17.62
	HETATM	3837	C4	DES	B	600	-1.433	-7.072	25.634	1.00	16.16
	HETATM	3838	C3	DES	B	600	-0.077	-6.685	25.542	1.00	20.04
	HETATM	3839	O3	DES	B	600	0.509	-6.113	26.655	1.00	15.55
	HETATM	3840	C2	DES	B	600	0.669	-6.866	24.353	1.00	18.94
40	HETATM	3841	C1	DES	B	600	0.035	-7.440	23.241	1.00	15.20
	HETATM	3842	C8	DES	B	600	-1.642	-9.903	21.942	1.00	17.61
	HETATM	3843	C9	DES	B	600	-0.440	-10.009	20.998	1.00	11.63
	HETATM	3844	C1	CBM	B	417	-4.997	-22.994	25.273	1.00	55.80
	HETATM	3845	O4	CBM	B	417	-4.789	-24.187	25.003	1.00	55.56
45	HETATM	3846	O3	CBM	B	417	-4.798	-22.559	26.552	1.00	56.04
	HETATM	3847	C2	CBM	B	417	-5.468	-21.960	24.264	1.00	57.04
	HETATM	3848	C1	CBM	B	530	-15.278	-5.124	10.243	1.00	87.39
	HETATM	3849	O4	CBM	B	530	-15.852	-5.086	9.064	1.00	87.68
	HETATM	3850	O3	CBM	B	530	-15.832	-4.291	11.201	1.00	86.22
50	HETATM	3851	C2	CBM	B	530	-14.207	-5.886	10.628	1.00	87.65
	ATOM	3852	CB	HIS	C	687	9.818	-20.030	-2.211	1.00	63.34
	ATOM	3853	C	HIS	C	687	10.133	-20.267	-4.689	1.00	63.49
	ATOM	3854	O	HIS	C	687	11.204	-20.840	-4.472	1.00	63.87
	ATOM	3855	N	HIS	C	687	7.944	-19.563	-3.758	1.00	65.42
55	ATOM	3856	CA	HIS	C	687	9.424	-19.484	-3.586	1.00	64.86
	ATOM	3857	N	LYS	C	688	9.533	-20.281	-5.875	1.00	62.00
	ATOM	3858	CA	LYS	C	688	10.101	-20.999	-7.009	1.00	60.81
	ATOM	3859	CB	LYS	C	688	8.980	-21.540	-7.901	1.00	61.76
	ATOM	3860	C	LYS	C	688	11.050	-20.127	-7.827	1.00	57.47
60	ATOM	3861	O	LYS	C	688	12.253	-20.379	-7.858	1.00	57.64
	ATOM	3862	N	ILE	C	689	10.511	-19.103	-8.482	1.00	55.74

5	ATOM	3863	CA	ILE	C	689	11.326	-18.212	-9.306	1.00	53.09
	ATOM	3864	CB	ILE	C	689	10.496	-17.057	-9.889	1.00	53.83
	ATOM	3865	CG2	ILE	C	689	11.334	-16.286	-10.902	1.00	54.55
	ATOM	3866	CG1	ILE	C	689	9.229	-17.603	-10.551	1.00	52.90
	ATOM	3867	CD1	ILE	C	689	8.406	-16.550	-11.258	1.00	50.45
10	ATOM	3868	C	ILE	C	689	12.513	-17.611	-8.560	1.00	50.82
	ATOM	3869	O	ILE	C	689	13.616	-17.550	-9.097	1.00	51.28
	ATOM	3870	N	LEU	C	690	12.288	-17.162	-7.329	1.00	48.01
	ATOM	3871	CA	LEU	C	690	13.362	-16.570	-6.534	1.00	47.33
	ATOM	3872	CB	LEU	C	690	12.812	-16.058	-5.199	1.00	42.51
15	ATOM	3873	CG	LEU	C	690	13.835	-15.501	-4.206	1.00	40.67
	ATOM	3874	CD1	LEU	C	690	14.575	-14.324	-4.831	1.00	39.95
	ATOM	3875	CD2	LEU	C	690	13.128	-15.078	-2.926	1.00	38.77
	ATOM	3876	C	LEU	C	690	14.445	-17.615	-6.282	1.00	48.87
	ATOM	3877	O	LEU	C	690	15.643	-17.340	-6.393	1.00	46.71
20	ATOM	3878	N	HIS	C	691	14.001	-18.818	-5.939	1.00	51.36
	ATOM	3879	CA	HIS	C	691	14.886	-19.946	-5.675	1.00	53.35
	ATOM	3880	CB	HIS	C	691	14.042	-21.203	-5.460	1.00	58.64
	ATOM	3881	CG	HIS	C	691	14.655	-22.195	-4.526	1.00	62.94
	ATOM	3882	CD2	HIS	C	691	15.503	-23.227	-4.751	1.00	64.95
25	ATOM	3883	ND1	HIS	C	691	14.392	-22.202	-3.173	1.00	65.49
	ATOM	3884	CE1	HIS	C	691	15.053	-23.195	-2.605	1.00	68.18
	ATOM	3885	NE2	HIS	C	691	15.733	-23.833	-3.540	1.00	68.77
	ATOM	3886	C	HIS	C	691	15.824	-20.162	-6.861	1.00	52.19
	ATOM	3887	O	HIS	C	691	17.048	-20.153	-6.717	1.00	47.53
30	ATOM	3888	N	ARG	C	692	15.222	-20.350	-8.032	1.00	52.37
	ATOM	3889	CA	ARG	C	692	15.949	-20.586	-9.271	1.00	52.90
	ATOM	3890	CB	ARG	C	692	14.955	-20.832	-10.410	1.00	54.04
	ATOM	3891	CG	ARG	C	692	15.575	-20.826	-11.797	1.00	57.52
	ATOM	3892	CD	ARG	C	692	14.528	-21.048	-12.874	1.00	58.25
35	ATOM	3893	NE	ARG	C	692	14.375	-19.878	-13.732	1.00	61.43
	ATOM	3894	CZ	ARG	C	692	13.218	-19.260	-13.951	1.00	64.32
	ATOM	3895	NH1	ARG	C	692	12.108	-19.706	-13.378	1.00	63.22
	ATOM	3896	NH2	ARG	C	692	13.171	-18.197	-14.746	1.00	65.93
	ATOM	3897	C	ARG	C	692	16.873	-19.434	-9.639	1.00	53.09
40	ATOM	3898	O	ARG	C	692	18.047	-19.644	-9.956	1.00	53.06
	ATOM	3899	N	LEU	C	693	16.338	-18.217	-9.607	1.00	50.73
	ATOM	3900	CA	LEU	C	693	17.125	-17.039	-9.945	1.00	49.53
	ATOM	3901	CB	LEU	C	693	16.249	-15.784	-9.881	1.00	49.56
	ATOM	3902	CG	LEU	C	693	15.781	-15.245	-11.239	1.00	49.78
45	ATOM	3903	CD1	LEU	C	693	15.219	-16.389	-12.079	1.00	50.30
	ATOM	3904	CD2	LEU	C	693	14.728	-14.170	-11.037	1.00	48.79
	ATOM	3905	C	LEU	C	693	18.318	-16.904	-9.006	1.00	48.38
	ATOM	3906	O	LEU	C	693	19.382	-16.426	-9.402	1.00	46.35
	ATOM	3907	N	LEU	C	694	18.135	-17.329	-7.761	1.00	46.74
50	ATOM	3908	CA	LEU	C	694	19.204	-17.272	-6.775	1.00	49.41
	ATOM	3909	CB	LEU	C	694	18.634	-17.415	-5.362	1.00	45.20
	ATOM	3910	CG	LEU	C	694	18.222	-16.128	-4.643	1.00	40.19
	ATOM	3911	CD1	LEU	C	694	17.456	-16.474	-3.371	1.00	41.65
	ATOM	3912	CD2	LEU	C	694	19.453	-15.307	-4.317	1.00	35.91
55	ATOM	3913	C	LEU	C	694	20.172	-18.417	-7.058	1.00	54.15
	ATOM	3914	O	LEU	C	694	21.370	-18.320	-6.776	1.00	53.55
	ATOM	3915	N	GLN	C	695	19.634	-19.498	-7.619	1.00	57.44
	ATOM	3916	CA	GLN	C	695	20.416	-20.685	-7.959	1.00	62.46
	ATOM	3917	CB	GLN	C	695	19.477	-21.853	-8.304	1.00	61.95
60	ATOM	3918	CG	GLN	C	695	19.548	-23.010	-7.311	1.00	61.49
	ATOM	3919	CD	GLN	C	695	18.454	-24.053	-7.490	1.00	62.78

5	ATOM	3920	OE1	GLN	C	695	18.262	-24.928	-6.653	1.00	63.33
	ATOM	3921	NE2	GLN	C	695	17.720	-23.969	-8.608	1.00	60.37
	ATOM	3922	C	GLN	C	695	21.330	-20.414	-9.149	1.00	65.13
	ATOM	3923	O	GLN	C	695	22.517	-20.740	-9.116	1.00	65.87
	ATOM	3924	N	ASP	C	696	20.761	-19.824	-10.197	1.00	67.67
10	ATOM	3925	CA	ASP	C	696	21.492	-19.500	-11.420	1.00	70.66
	ATOM	3926	CB	ASP	C	696	20.801	-18.348	-12.151	1.00	71.06
	ATOM	3927	CG	ASP	C	696	20.127	-18.792	-13.430	1.00	71.70
	ATOM	3928	OD1	ASP	C	696	20.637	-18.455	-14.521	1.00	72.47
	ATOM	3929	OD2	ASP	C	696	19.086	-19.478	-13.342	1.00	71.41
15	ATOM	3930	C	ASP	C	696	22.951	-19.132	-11.169	1.00	72.41
	ATOM	3931	O	ASP	C	696	23.245	-18.115	-10.541	1.00	72.56
	ATOM	3932	N	SER	C	697	23.859	-19.967	-11.668	1.00	74.67
	ATOM	3933	CA	SER	C	697	25.291	-19.741	-11.507	1.00	76.45
	ATOM	3934	CB	SER	C	697	26.019	-21.076	-11.377	1.00	76.00
20	ATOM	3935	C	SER	C	697	25.841	-18.960	-12.696	1.00	78.44
	ATOM	3936	O	SER	C	697	26.286	-17.809	-12.489	1.00	79.20
	ATOM	3937	OXT	SER	C	697	25.818	-19.510	-13.820	1.00	80.07
	ATOM	3938	CB	LYS	D	686	-14.070	13.661	16.843	1.00	50.28
	ATOM	3939	C	LYS	D	686	-13.682	14.418	19.199	1.00	51.59
25	ATOM	3940	O	LYS	D	686	-12.629	14.738	19.759	1.00	50.42
	ATOM	3941	N	LYS	D	686	-12.910	15.796	17.283	1.00	50.43
	ATOM	3942	CA	LYS	D	686	-13.976	14.872	17.769	1.00	50.62
	ATOM	3943	N	HIS	D	687	-14.617	13.676	19.787	1.00	49.91
	ATOM	3944	CA	HIS	D	687	-14.447	13.176	21.144	1.00	51.28
30	ATOM	3945	CB	HIS	D	687	-15.806	12.984	21.828	1.00	54.12
	ATOM	3946	CG	HIS	D	687	-15.713	12.336	23.177	1.00	60.06
	ATOM	3947	CD2	HIS	D	687	-15.418	11.064	23.539	1.00	61.05
	ATOM	3948	ND1	HIS	D	687	-15.911	13.030	24.352	1.00	62.39
	ATOM	3949	CE1	HIS	D	687	-15.741	12.215	25.378	1.00	62.76
35	ATOM	3950	NE2	HIS	D	687	-15.441	11.016	24.912	1.00	63.46
	ATOM	3951	C	HIS	D	687	-13.691	11.849	21.163	1.00	49.55
	ATOM	3952	O	HIS	D	687	-14.099	10.878	20.524	1.00	50.84
	ATOM	3953	N	LYS	D	688	-12.593	11.816	21.909	1.00	44.00
	ATOM	3954	CA	LYS	D	688	-11.784	10.611	22.038	1.00	40.31
40	ATOM	3955	CB	LYS	D	688	-10.446	10.773	21.299	1.00	41.42
	ATOM	3956	CG	LYS	D	688	-10.513	10.595	19.780	1.00	42.76
	ATOM	3957	CD	LYS	D	688	-9.123	10.716	19.152	1.00	38.65
	ATOM	3958	CE	LYS	D	688	-9.162	10.529	17.640	1.00	38.28
	ATOM	3959	NZ	LYS	D	688	-7.894	10.970	16.986	1.00	31.58
45	ATOM	3960	C	LYS	D	688	-11.506	10.378	23.517	1.00	36.70
	ATOM	3961	O	LYS	D	688	-11.271	11.326	24.266	1.00	33.38
	ATOM	3962	N	ILE	D	689	-11.549	9.122	23.942	1.00	33.06
	ATOM	3963	CA	ILE	D	689	-11.255	8.806	25.328	1.00	28.70
	ATOM	3964	CB	ILE	D	689	-11.438	7.301	25.607	1.00	30.88
50	ATOM	3965	CG2	ILE	D	689	-10.725	6.912	26.899	1.00	31.45
	ATOM	3966	CG1	ILE	D	689	-12.927	6.971	25.721	1.00	32.57
	ATOM	3967	CD1	ILE	D	689	-13.308	5.679	25.031	1.00	29.79
	ATOM	3968	C	ILE	D	689	-9.790	9.193	25.541	1.00	27.64
	ATOM	3969	O	ILE	D	689	-9.405	9.649	26.611	1.00	25.54
55	ATOM	3970	N	LEU	D	690	-8.985	9.021	24.496	1.00	24.25
	ATOM	3971	CA	LEU	D	690	-7.563	9.348	24.549	1.00	26.63
	ATOM	3972	CB	LEU	D	690	-6.903	9.021	23.200	1.00	22.83
	ATOM	3973	CG	LEU	D	690	-5.433	9.387	22.992	1.00	25.47
	ATOM	3974	CD1	LEU	D	690	-4.595	8.772	24.108	1.00	24.03
60	ATOM	3975	CD2	LEU	D	690	-4.956	8.898	21.616	1.00	20.87
	ATOM	3976	C	LEU	D	690	-7.344	10.823	24.902	1.00	26.64

5	ATOM	3977	O	LEU	D	690	-6.408	11.165	25.625	1.00	28.34
	ATOM	3978	N	HIS	D	691	-8.206	11.694	24.383	1.00	27.77
	ATOM	3979	CA	HIS	D	691	-8.107	13.125	24.665	1.00	29.16
	ATOM	3980	CB	HIS	D	691	-9.156	13.907	23.861	1.00	30.89
	ATOM	3981	CG	HIS	D	691	-8.903	13.935	22.386	1.00	37.09
10	ATOM	3982	CD2	HIS	D	691	-7.750	14.000	21.679	1.00	41.39
	ATOM	3983	ND1	HIS	D	691	-9.920	13.906	21.458	1.00	41.65
	ATOM	3984	CE1	HIS	D	691	-9.407	13.953	20.242	1.00	44.64
	ATOM	3985	NE2	HIS	D	691	-8.091	14.010	20.347	1.00	41.94
	ATOM	3986	C	HIS	D	691	-8.338	13.373	26.159	1.00	26.65
15	ATOM	3987	O	HIS	D	691	-7.602	14.120	26.802	1.00	24.50
	ATOM	3988	N	ARG	D	692	-9.371	12.742	26.703	1.00	25.70
	ATOM	3989	CA	ARG	D	692	-9.691	12.912	28.114	1.00	29.11
	ATOM	3990	CB	ARG	D	692	-10.959	12.134	28.472	1.00	30.84
	ATOM	3991	CG	ARG	D	692	-11.255	12.129	29.963	1.00	41.63
20	ATOM	3992	CD	ARG	D	692	-12.502	11.327	30.290	1.00	48.83
	ATOM	3993	NE	ARG	D	692	-13.618	12.198	30.647	1.00	54.50
	ATOM	3994	CZ	ARG	D	692	-14.498	12.677	29.774	1.00	59.37
	ATOM	3995	NH1	ARG	D	692	-14.392	12.371	28.486	1.00	60.97
	ATOM	3996	NH2	ARG	D	692	-15.483	13.464	30.188	1.00	59.07
25	ATOM	3997	C	ARG	D	692	-8.548	12.451	29.011	1.00	28.30
	ATOM	3998	O	ARG	D	692	-8.139	13.167	29.929	1.00	26.50
	ATOM	3999	N	LEU	D	693	-8.030	11.259	28.737	1.00	24.87
	ATOM	4000	CA	LEU	D	693	-6.943	10.705	29.536	1.00	27.17
	ATOM	4001	CB	LEU	D	693	-6.674	9.254	29.116	1.00	28.45
30	ATOM	4002	CG	LEU	D	693	-7.844	8.300	29.391	1.00	30.40
	ATOM	4003	CD1	LEU	D	693	-7.575	6.932	28.778	1.00	34.79
	ATOM	4004	CD2	LEU	D	693	-8.043	8.171	30.894	1.00	32.02
	ATOM	4005	C	LEU	D	693	-5.670	11.539	29.440	1.00	25.96
	ATOM	4006	O	LEU	D	693	-4.948	11.700	30.428	1.00	27.01
35	ATOM	4007	N	LEU	D	694	-5.395	12.080	28.257	1.00	25.33
	ATOM	4008	CA	LEU	D	694	-4.207	12.906	28.062	1.00	27.22
	ATOM	4009	CB	LEU	D	694	-3.948	13.126	26.572	1.00	24.61
	ATOM	4010	CG	LEU	D	694	-3.118	12.080	25.825	1.00	22.20
	ATOM	4011	CD1	LEU	D	694	-3.230	12.332	24.324	1.00	21.13
40	ATOM	4012	CD2	LEU	D	694	-1.666	12.148	26.275	1.00	21.34
	ATOM	4013	C	LEU	D	694	-4.336	14.270	28.742	1.00	32.40
	ATOM	4014	O	LEU	D	694	-3.339	14.889	29.102	1.00	31.55
	ATOM	4015	N	GLN	D	695	-5.570	14.733	28.915	1.00	36.93
	ATOM	4016	CA	GLN	D	695	-5.820	16.032	29.528	1.00	43.18
45	ATOM	4017	CB	GLN	D	695	-7.022	16.694	28.862	1.00	40.48
	ATOM	4018	CG	GLN	D	695	-6.772	17.071	27.422	1.00	37.99
	ATOM	4019	CD	GLN	D	695	-7.943	17.764	26.795	1.00	35.86
	ATOM	4020	OE1	GLN	D	695	-7.863	18.895	26.342	1.00	38.84
	ATOM	4021	NE2	GLN	D	695	-9.082	17.060	26.757	1.00	31.62
50	ATOM	4022	C	GLN	D	695	-6.049	16.009	31.034	1.00	48.74
	ATOM	4023	O	GLN	D	695	-6.119	17.065	31.660	1.00	51.25
	ATOM	4024	N	ASP	D	696	-6.175	14.818	31.611	1.00	54.01
	ATOM	4025	CA	ASP	D	696	-6.398	14.702	33.047	1.00	62.23
	ATOM	4026	CB	ASP	D	696	-6.217	13.238	33.485	1.00	63.97
55	ATOM	4027	CG	ASP	D	696	-7.527	12.467	33.475	1.00	67.72
	ATOM	4028	OD1	ASP	D	696	-8.528	12.996	32.941	1.00	68.11
	ATOM	4029	OD2	ASP	D	696	-7.552	11.333	34.003	1.00	68.95
	ATOM	4030	C	ASP	D	696	-5.456	15.622	33.840	1.00	65.60
	ATOM	4031	O	ASP	D	696	-4.312	15.189	34.134	1.00	68.33
60	ATOM	4032	OXT	ASP	D	696	-5.874	16.755	34.140	1.00	69.20
	HETATM	4033	O	HOH		1	16.153	-0.605	-4.425	1.00	17.11

5	HETATM	4034	O	HOH	2	16.570	-5.304	-16.560	1.00	21.44
	HETATM	4035	O	HOH	3	18.526	0.742	-4.495	1.00	23.43
	HETATM	4036	O	HOH	4	13.647	-2.187	8.588	1.00	25.82
	HETATM	4037	O	HOH	5	9.778	-5.825	2.509	1.00	20.58
	HETATM	4038	O	HOH	6	17.072	-3.605	-8.015	1.00	18.38
10	HETATM	4039	O	HOH	7	24.920	-1.689	-2.780	1.00	25.74
	HETATM	4040	O	HOH	8	7.321	-5.649	5.061	1.00	24.11
	HETATM	4041	O	HOH	9	25.976	-3.535	15.158	1.00	26.78
	HETATM	4042	O	HOH	10	15.088	-7.006	-15.192	1.00	19.64
	HETATM	4043	O	HOH	11	14.070	0.925	-5.953	1.00	20.55
15	HETATM	4044	O	HOH	12	18.008	3.407	-6.654	1.00	32.30
	HETATM	4045	O	HOH	13	31.949	-8.393	13.487	1.00	30.64
	HETATM	4046	O	HOH	14	19.625	-2.804	-4.279	1.00	24.45
	HETATM	4047	O	HOH	15	11.741	1.079	-21.140	1.00	25.87
	HETATM	4048	O	HOH	16	25.067	13.951	14.153	1.00	31.07
20	HETATM	4049	O	HOH	17	15.501	1.323	-10.393	1.00	21.01
	HETATM	4050	O	HOH	18	13.880	3.349	-11.482	1.00	24.28
	HETATM	4051	O	HOH	19	17.591	0.979	-8.828	1.00	35.26
	HETATM	4052	O	HOH	20	23.682	-2.041	-0.314	1.00	37.90
	HETATM	4053	O	HOH	21	15.754	9.496	11.841	1.00	39.44
25	HETATM	4054	O	HOH	22	-4.943	7.574	-3.066	1.00	37.67
	HETATM	4055	O	HOH	23	6.877	0.354	-15.982	1.00	36.92
	HETATM	4056	O	HOH	24	15.806	-4.002	8.671	1.00	30.38
	HETATM	4057	O	HOH	25	17.185	-3.158	-5.321	1.00	28.89
	HETATM	4058	O	HOH	26	17.572	9.249	17.009	1.00	30.15
30	HETATM	4059	O	HOH	27	24.096	-2.929	11.604	1.00	31.37
	HETATM	4060	O	HOH	28	22.324	-5.871	-11.980	1.00	32.74
	HETATM	4061	O	HOH	29	27.547	-12.361	-0.801	1.00	36.61
	HETATM	4062	O	HOH	30	11.173	13.442	-2.719	1.00	35.41
	HETATM	4063	O	HOH	31	15.438	-9.527	5.483	1.00	29.88
35	HETATM	4064	O	HOH	32	9.946	-6.564	5.983	1.00	35.05
	HETATM	4065	O	HOH	33	7.599	11.680	-15.261	1.00	38.68
	HETATM	4066	O	HOH	34	20.112	10.503	-5.109	1.00	42.66
	HETATM	4067	O	HOH	35	15.972	10.343	14.897	1.00	41.73
	HETATM	4068	O	HOH	36	22.401	-5.914	-9.527	1.00	28.08
40	HETATM	4069	O	HOH	37	16.128	-0.899	-8.109	1.00	33.13
	HETATM	4070	O	HOH	38	3.581	15.655	-3.706	1.00	41.37
	HETATM	4071	O	HOH	39	31.900	13.545	21.339	1.00	37.79
	HETATM	4072	O	HOH	40	20.058	-7.530	14.119	1.00	47.51
	HETATM	4073	O	HOH	41	34.634	6.668	15.632	1.00	29.24
45	HETATM	4074	O	HOH	42	17.968	10.511	-9.085	1.00	44.60
	HETATM	4075	O	HOH	43	23.258	-17.325	-4.088	1.00	44.10
	HETATM	4076	O	HOH	44	4.034	-1.472	27.521	1.00	15.22
	HETATM	4077	O	HOH	45	-5.943	-0.018	36.088	1.00	21.11
	HETATM	4078	O	HOH	46	6.084	-1.509	29.478	1.00	19.51
50	HETATM	4079	O	HOH	47	9.762	1.061	15.621	1.00	27.74
	HETATM	4080	O	HOH	48	1.804	0.717	17.260	1.00	20.97
	HETATM	4081	O	HOH	49	0.929	0.421	30.281	1.00	19.64
	HETATM	4082	O	HOH	50	9.627	4.271	31.231	1.00	19.02
	HETATM	4083	O	HOH	51	2.121	-0.261	13.654	1.00	26.09
55	HETATM	4084	O	HOH	52	20.060	10.275	17.711	1.00	25.49
	HETATM	4085	O	HOH	53	-6.786	0.736	33.483	1.00	22.34
	HETATM	4086	O	HOH	54	2.751	-4.136	27.760	1.00	19.93
	HETATM	4087	O	HOH	55	5.994	-4.079	31.292	1.00	32.27
	HETATM	4088	O	HOH	56	19.416	16.921	21.645	1.00	25.54
60	HETATM	4089	O	HOH	57	4.833	2.325	29.006	1.00	19.00
	HETATM	4090	O	HOH	58	-7.638	-8.931	37.809	1.00	24.79

5	HETATM	4091	O	HOH	59	28.442	-4.673	21.875	1.00	24.32
	HETATM	4092	O	HOH	60	1.094	-4.893	32.100	1.00	24.27
	HETATM	4093	O	HOH	61	0.905	-7.306	32.783	1.00	21.33
	HETATM	4094	O	HOH	62	3.396	-2.971	32.306	1.00	26.13
	HETATM	4095	O	HOH	63	10.363	4.576	28.391	1.00	33.43
10	HETATM	4096	O	HOH	64	19.551	-6.473	16.597	1.00	35.38
	HETATM	4097	O	HOH	65	-2.888	-19.627	15.665	1.00	27.99
	HETATM	4098	O	HOH	66	-7.275	-9.745	31.077	1.00	27.00
	HETATM	4099	O	HOH	67	10.189	3.580	16.510	1.00	24.19
	HETATM	4100	O	HOH	68	2.741	0.716	28.382	1.00	16.48
15	HETATM	4101	O	HOH	69	23.522	-4.323	13.943	1.00	27.48
	HETATM	4102	O	HOH	70	17.133	8.133	19.686	1.00	32.24
	HETATM	4103	O	HOH	71	-0.295	4.535	35.884	1.00	33.42
	HETATM	4104	O	HOH	72	9.519	10.828	34.842	1.00	29.38
	HETATM	4105	O	HOH	73	6.291	14.878	29.070	1.00	28.21
20	HETATM	4106	O	HOH	74	-1.721	6.480	13.381	1.00	49.91
	HETATM	4107	O	HOH	75	10.091	-15.427	26.194	1.00	24.17
	HETATM	4108	O	HOH	76	5.029	7.461	17.718	1.00	18.91
	HETATM	4109	O	HOH	77	3.758	2.086	14.306	1.00	28.28
	HETATM	4110	O	HOH	78	-1.390	-18.739	33.183	1.00	41.11
25	HETATM	4111	O	HOH	79	12.703	-8.687	32.119	1.00	36.21
	HETATM	4112	O	HOH	80	22.270	-6.451	14.844	1.00	33.21
	HETATM	4113	O	HOH	81	1.458	4.605	34.026	1.00	23.59
	HETATM	4114	O	HOH	82	1.759	-2.158	30.374	1.00	28.78
	HETATM	4115	O	HOH	83	6.153	-21.372	23.188	1.00	31.14
30	HETATM	4116	O	HOH	84	36.525	0.463	20.792	1.00	45.26
	HETATM	4117	O	HOH	85	13.832	9.696	13.792	1.00	33.12
	HETATM	4118	O	HOH	86	31.166	6.635	24.924	1.00	35.19
	HETATM	4119	O	HOH	87	8.844	-10.389	34.180	1.00	48.80
	HETATM	4120	O	HOH	88	9.581	-6.956	34.136	1.00	42.95
35	HETATM	4121	O	HOH	89	-1.563	15.887	27.596	1.00	39.35
	HETATM	4122	O	HOH	90	-5.286	10.345	32.757	1.00	35.20
	HETATM	4123	O	HOH	91	15.035	0.607	13.339	1.00	29.53
	HETATM	4124	O	HOH	92	-10.984	-1.500	30.272	1.00	29.84
	HETATM	4125	O	HOH	93	-7.239	-0.271	-1.207	1.00	48.98
40	HETATM	4126	O	HOH	94	18.022	-4.902	34.286	1.00	35.28
	HETATM	4127	O	HOH	95	29.347	-6.319	19.920	1.00	37.20
	HETATM	4128	O	HOH	96	-14.309	-19.369	20.945	1.00	30.23
	HETATM	4129	O	HOH	97	31.496	4.614	18.716	1.00	38.79
	HETATM	4130	O	HOH	98	26.567	9.759	25.629	1.00	29.72
45	HETATM	4131	O	HOH	99	2.848	14.531	1.134	1.00	38.08
	HETATM	4132	O	HOH	100	-9.373	5.699	-7.953	1.00	53.23
	HETATM	4133	O	HOH	101	-10.137	-0.553	-6.742	1.00	47.72
	HETATM	4134	O	HOH	102	10.558	-10.363	15.403	1.00	40.97



5	HETATM	4148	O	HOH	116	7.170	15.583	2.599	1.00	43.69
	HETATM	4149	O	HOH	117	-1.966	10.606	3.572	1.00	52.63
	HETATM	4150	O	HOH	118	29.030	10.644	6.707	1.00	42.54
	HETATM	4151	O	HOH	119	0.468	4.354	8.374	1.00	38.69
	HETATM	4152	O	HOH	120	29.086	17.119	19.272	1.00	45.51
10	HETATM	4153	O	HOH	121	24.614	17.609	20.174	1.00	53.55
	HETATM	4154	O	HOH	122	-15.318	0.362	26.686	1.00	36.77
	HETATM	4155	O	HOH	123	-3.857	-24.786	28.325	1.00	39.64
	HETATM	4156	O	HOH	124	21.728	22.178	31.983	1.00	43.73
	HETATM	4157	O	HOH	125	31.650	-7.370	21.642	1.00	40.53
15	HETATM	4158	O	HOH	126	25.421	10.436	21.161	1.00	32.31
	HETATM	4159	O	HOH	127	10.317	-9.457	12.998	1.00	37.77
	HETATM	4160	O	HOH	128	22.723	14.887	15.427	1.00	47.90
	HETATM	4161	O	HOH	129	6.702	9.556	37.596	1.00	47.81
	HETATM	4162	O	HOH	130	27.987	13.557	7.167	1.00	41.15
20	HETATM	4163	O	HOH	131	30.798	16.499	7.588	1.00	58.47
	HETATM	4164	O	HOH	132	10.071	-0.571	-20.393	1.00	38.79
	HETATM	4165	O	HOH	133	9.562	8.334	-21.392	1.00	36.80
	HETATM	4166	O	HOH	134	6.712	6.058	8.822	1.00	37.43
	HETATM	4167	O	HOH	135	5.927	8.454	10.594	1.00	42.34
25	HETATM	4168	O	HOH	136	4.472	6.306	10.973	1.00	37.35
	HETATM	4169	O	HOH	137	6.792	7.721	7.051	1.00	47.23
	HETATM	4170	O	HOH	138	24.513	11.582	33.724	1.00	45.55
	HETATM	4171	O	HOH	139	-2.528	-20.361	12.354	1.00	52.13
	HETATM	4172	O	HOH	140	-7.864	7.706	19.248	1.00	47.82
30	HETATM	4173	O	HOH	141	11.577	-16.962	24.398	1.00	39.43
	HETATM	4174	O	HOH	142	18.087	12.263	-5.507	1.00	33.36
	HETATM	4175	O	HOH	143	-6.816	-14.190	10.674	1.00	51.32
	HETATM	4176	O	HOH	144	-7.377	-16.701	33.528	1.00	57.11
	HETATM	4177	O	HOH	145	-5.379	-20.107	32.689	1.00	43.01
35	HETATM	4178	O	HOH	146	8.766	-7.947	-16.274	1.00	49.96
	HETATM	4179	O	HOH	147	10.946	-7.937	-18.142	1.00	55.67
	END									

5

## Appendix 3

Atomic Coordinates for Human ER $\alpha$  Complexed With OHT

	CRYST1	58.242	58.242	277.467	90.00	90.00	120.00	P	65	2	2	12
10	ORIGX1	1.000000	0.000000	0.000000	0.000000							
	ORIGX2	0.000000	1.000000	0.000000	0.000000							
	ORIGX3	0.000000	0.000000	1.000000	0.000000							
	SCALE1	0.017170	0.009913	0.000000	0.000000							
15	SCALE2	0.000000	0.019826	0.000000	0.000000							
	SCALE3	0.000000	0.000000	0.003604	0.000000							
	ATOM	1	CB	LEU	306	6.638	11.502	3.989	1.00	61.20		
	ATOM	2	C	LEU	306	7.381	10.684	6.231	1.00	61.47		
20	ATOM	3	O	LEU	306	6.407	11.020	6.905	1.00	62.09		
	ATOM	4	N	LEU	306	6.369	9.128	4.588	1.00	62.32		
	ATOM	5	CA	LEU	306	7.232	10.330	4.754	1.00	61.30		
	ATOM	6	N	ALA	307	8.609	10.605	6.730	1.00	60.52		
	ATOM	7	CA	ALA	307	8.891	10.912	8.125	1.00	58.77		
25	ATOM	8	CB	ALA	307	10.318	10.501	8.465	1.00	59.70		
	ATOM	9	C	ALA	307	8.692	12.393	8.429	1.00	57.51		
	ATOM	10	O	ALA	307	8.451	12.770	9.574	1.00	57.64		
	ATOM	11	N	LEU	308	8.789	13.228	7.400	1.00	55.82		
	ATOM	12	CA	LEU	308	8.638	14.668	7.573	1.00	56.62		
30	ATOM	13	CB	LEU	308	9.298	15.402	6.406	1.00	57.48		
	ATOM	14	CG	LEU	308	10.637	14.822	5.948	1.00	59.17		
	ATOM	15	CD1	LEU	308	10.474	14.189	4.569	1.00	60.38		
	ATOM	16	CD2	LEU	308	11.694	15.920	5.933	1.00	58.46		
	ATOM	17	C	LEU	308	7.190	15.130	7.710	1.00	56.51		
35	ATOM	18	O	LEU	308	6.935	16.307	7.961	1.00	55.58		
	ATOM	19	N	SER	309	6.246	14.208	7.546	1.00	57.04		
	ATOM	20	CA	SER	309	4.828	14.544	7.657	1.00	56.46		
	ATOM	21	CB	SER	309	4.034	13.896	6.514	1.00	56.79		
	ATOM	22	OG	SER	309	4.071	12.479	6.588	1.00	57.23		
40	ATOM	23	C	SER	309	4.261	14.095	9.003	1.00	56.13		
	ATOM	24	O	SER	309	3.166	14.507	9.398	1.00	55.17		
	ATOM	25	N	LEU	310	5.016	13.257	9.706	1.00	54.31		
	ATOM	26	CA	LEU	310	4.591	12.749	11.004	1.00	53.55		
	ATOM	27	CB	LEU	310	5.651	11.811	11.582	1.00	54.40		
45	ATOM	28	CG	LEU	310	5.586	10.333	11.189	1.00	56.49		
	ATOM	29	CD1	LEU	310	5.530	10.200	9.676	1.00	57.06		
	ATOM	30	CD2	LEU	310	6.809	9.610	11.739	1.00	57.28		
	ATOM	31	C	LEU	310	4.330	13.865	12.003	1.00	53.18		
	ATOM	32	O	LEU	310	4.993	14.905	11.984	1.00	53.17		
50	ATOM	33	N	THR	311	3.352	13.641	12.874	1.00	51.71		
	ATOM	34	CA	THR	311	3.017	14.604	13.912	1.00	49.93		
	ATOM	35	CB	THR	311	1.527	14.554	14.275	1.00	48.96		
	ATOM	36	OG1	THR	311	1.242	13.311	14.930	1.00	47.20		
	ATOM	37	CG2	THR	311	0.666	14.688	13.027	1.00	50.99		
55	ATOM	38	C	THR	311	3.815	14.201	15.145	1.00	48.84		
	ATOM	39	O	THR	311	4.371	13.103	15.197	1.00	46.66		
	ATOM	40	N	ALA	312	3.857	15.078	16.141	1.00	48.76		
	ATOM	41	CA	ALA	312	4.590	14.798	17.369	1.00	47.75		
	ATOM	42	CB	ALA	312	4.359	15.910	18.378	1.00	47.06		
60	ATOM	43	C	ALA	312	4.171	13.460	17.964	1.00	47.41		

5	ATOM	44	O	ALA	312	5.009	12.609	18.262	1.00	45.52
	ATOM	45	N	ASP	313	2.868	13.275	18.143	1.00	47.58
	ATOM	46	CA	ASP	313	2.367	12.032	18.714	1.00	47.63
	ATOM	47	CB	ASP	313	0.848	12.100	18.879	1.00	51.96
	ATOM	48	CG	ASP	313	0.430	12.872	20.118	1.00	56.21
10	ATOM	49	OD1	ASP	313	1.314	13.234	20.929	1.00	56.38
	ATOM	50	OD2	ASP	313	-0.785	13.117	20.282	1.00	59.15
	ATOM	51	C	ASP	313	2.745	10.846	17.835	1.00	43.93
	ATOM	52	O	ASP	313	2.959	9.741	18.330	1.00	44.77
	ATOM	53	N	GLN	314	2.826	11.081	16.531	1.00	44.52
15	ATOM	54	CA	GLN	314	3.182	10.028	15.588	1.00	44.73
	ATOM	55	CB	GLN	314	2.849	10.464	14.156	1.00	45.05
	ATOM	56	CG	GLN	314	1.534	9.886	13.626	1.00	48.47
	ATOM	57	CD	GLN	314	0.982	10.646	12.428	1.00	50.37
	ATOM	58	OE1	GLN	314	1.649	11.515	11.856	1.00	49.38
20	ATOM	59	NE2	GLN	314	-0.248	10.318	12.043	1.00	51.74
	ATOM	60	C	GLN	314	4.673	9.722	15.707	1.00	43.26
	ATOM	61	O	GLN	314	5.100	8.580	15.555	1.00	43.93
	ATOM	62	N	MET	315	5.459	10.757	15.980	1.00	42.29
	ATOM	63	CA	MET	315	6.901	10.606	16.130	1.00	41.26
25	ATOM	64	CB	MET	315	7.565	11.985	16.224	1.00	42.43
	ATOM	65	CG	MET	315	9.082	11.939	16.356	1.00	42.34
	ATOM	66	SD	MET	315	9.906	11.190	14.925	1.00	46.22
	ATOM	67	CE	MET	315	9.547	12.408	13.680	1.00	37.32
	ATOM	68	C	MET	315	7.218	9.791	17.379	1.00	38.89
30	ATOM	69	O	MET	315	8.002	8.841	17.335	1.00	40.02
	ATOM	70	N	VAL	316	6.599	10.165	18.491	1.00	37.65
	ATOM	71	CA	VAL	316	6.819	9.476	19.756	1.00	39.56
	ATOM	72	CB	VAL	316	6.023	10.136	20.897	1.00	39.22
	ATOM	73	CG1	VAL	316	6.245	9.373	22.192	1.00	44.43
35	ATOM	74	CG2	VAL	316	6.446	11.583	21.059	1.00	41.04
	ATOM	75	C	VAL	316	6.404	8.012	19.664	1.00	40.04
	ATOM	76	O	VAL	316	7.141	7.117	20.077	1.00	37.86
	ATOM	77	N	SER	317	5.215	7.767	19.127	1.00	41.90
	ATOM	78	CA	SER	317	4.733	6.400	18.997	1.00	41.68
40	ATOM	79	CB	SER	317	3.311	6.402	18.415	1.00	43.85
	ATOM	80	OG	SER	317	3.225	5.631	17.230	1.00	49.38
	ATOM	81	C	SER	317	5.696	5.601	18.114	1.00	39.72
	ATOM	82	O	SER	317	6.011	4.446	18.407	1.00	40.21
	ATOM	83	N	ALA	318	6.182	6.220	17.043	1.00	38.35
45	ATOM	84	CA	ALA	318	7.114	5.540	16.153	1.00	36.96
	ATOM	85	CB	ALA	318	7.485	6.448	14.986	1.00	37.92
	ATOM	86	C	ALA	318	8.375	5.137	16.920	1.00	38.31
	ATOM	87	O	ALA	318	8.820	3.992	16.844	1.00	33.94
	ATOM	88	N	LEU	319	8.938	6.089	17.664	1.00	36.92
50	ATOM	89	CA	LEU	319	10.161	5.854	18.438	1.00	38.56
	ATOM	90	CB	LEU	319	10.660	7.174	19.040	1.00	40.86
	ATOM	91	CG	LEU	319	11.136	8.264	18.071	1.00	41.25
	ATOM	92	CD1	LEU	319	11.714	9.440	18.857	1.00	44.30
	ATOM	93	CD2	LEU	319	12.182	7.693	17.140	1.00	42.61
55	ATOM	94	C	LEU	319	9.965	4.826	19.549	1.00	38.33
	ATOM	95	O	LEU	319	10.779	3.916	19.729	1.00	33.91
	ATOM	96	N	LEU	320	8.879	4.982	20.297	1.00	37.39
	ATOM	97	CA	LEU	320	8.567	4.067	21.387	1.00	41.55
	ATOM	98	CB	LEU	320	7.239	4.467	22.049	1.00	38.47
60	ATOM	99	CG	LEU	320	7.236	5.582	23.099	1.00	44.81
	ATOM	100	CD1	LEU	320	5.876	5.634	23.802	1.00	44.96

5	ATOM	101	CD2	LEU	320	8.334	5.332	24.112	1.00	43.36
	ATOM	102	C	LEU	320	8.466	2.642	20.843	1.00	41.11
	ATOM	103	O	LEU	320	8.971	1.697	21.443	1.00	41.87
	ATOM	104	N	ASP	321	7.812	2.504	19.696	1.00	43.94
	ATOM	105	CA	ASP	321	7.613	1.210	19.053	1.00	44.77
10	ATOM	106	CB	ASP	321	6.669	1.372	17.860	1.00	48.39
	ATOM	107	CG	ASP	321	5.206	1.318	18.255	1.00	52.39
	ATOM	108	OD1	ASP	321	4.901	1.422	19.464	1.00	53.56
	ATOM	109	OD2	ASP	321	4.357	1.172	17.346	1.00	55.81
	ATOM	110	C	ASP	321	8.911	0.565	18.568	1.00	44.37
15	ATOM	111	O	ASP	321	9.030	-0.661	18.533	1.00	44.67
	ATOM	112	N	ALA	322	9.878	1.395	18.193	1.00	40.75
	ATOM	113	CA	ALA	322	11.153	0.905	17.686	1.00	37.81
	ATOM	114	CB	ALA	322	11.772	1.954	16.776	1.00	38.07
	ATOM	115	C	ALA	322	12.148	0.513	18.769	1.00	35.52
20	ATOM	116	O	ALA	322	13.219	-0.020	18.473	1.00	36.11
	ATOM	117	N	GLU	323	11.799	0.768	20.022	1.00	35.61
	ATOM	118	CA	GLU	323	12.704	0.460	21.117	1.00	36.39
	ATOM	119	CB	GLU	323	12.042	0.768	22.459	1.00	35.09
	ATOM	120	CG	GLU	323	12.209	2.210	22.899	1.00	37.93
25	ATOM	121	CD	GLU	323	13.657	2.569	23.200	1.00	37.29
	ATOM	122	OE1	GLU	323	14.313	3.173	22.326	1.00	34.21
	ATOM	123	OE2	GLU	323	14.134	2.245	24.309	1.00	38.02
	ATOM	124	C	GLU	323	13.205	-0.978	21.110	1.00	38.01
	ATOM	125	O	GLU	323	12.425	-1.931	20.999	1.00	38.37
30	ATOM	126	N	PRO	324	14.527	-1.151	21.225	1.00	36.03
	ATOM	127	CD	PRO	324	15.522	-0.069	21.345	1.00	36.69
	ATOM	128	CA	PRO	324	15.158	-2.474	21.240	1.00	36.42
	ATOM	129	CB	PRO	324	16.633	-2.166	21.003	1.00	35.75
	ATOM	130	CG	PRO	324	16.811	-0.807	21.610	1.00	35.46
35	ATOM	131	C	PRO	324	14.940	-3.162	22.583	1.00	35.75
	ATOM	132	O	PRO	324	14.616	-2.517	23.580	1.00	34.97
	ATOM	133	N	PRO	325	15.134	-4.485	22.631	1.00	35.24
	ATOM	134	CD	PRO	325	15.530	-5.386	21.534	1.00	37.02
	ATOM	135	CA	PRO	325	14.942	-5.208	23.889	1.00	34.65
40	ATOM	136	CB	PRO	325	14.753	-6.652	23.439	1.00	35.83
	ATOM	137	CG	PRO	325	15.589	-6.743	22.200	1.00	34.88
	ATOM	138	C	PRO	325	16.132	-5.070	24.824	1.00	34.51
	ATOM	139	O	PRO	325	17.237	-4.723	24.399	1.00	29.92
	ATOM	140	N	ILE	326	15.899	-5.322	26.106	1.00	33.62
45	ATOM	141	CA	ILE	326	16.975	-5.265	27.075	1.00	35.02
	ATOM	142	CB	ILE	326	16.458	-4.891	28.473	1.00	38.11
	ATOM	143	CG2	ILE	326	17.557	-5.110	29.504	1.00	38.70
	ATOM	144	CG1	ILE	326	15.987	-3.431	28.466	1.00	40.48
	ATOM	145	CD1	ILE	326	16.035	-2.747	29.815	1.00	42.96
50	ATOM	146	C	ILE	326	17.567	-6.668	27.103	1.00	34.14
	ATOM	147	O	ILE	326	16.875	-7.634	27.427	1.00	34.88
	ATOM	148	N	LEU	327	18.840	-6.784	26.745	1.00	29.64
	ATOM	149	CA	LEU	327	19.493	-8.083	26.716	1.00	29.54
	ATOM	150	CB	LEU	327	20.528	-8.135	25.587	1.00	27.76
55	ATOM	151	CG	LEU	327	19.978	-7.800	24.196	1.00	29.02
	ATOM	152	CD1	LEU	327	21.068	-7.993	23.139	1.00	28.76
	ATOM	153	CD2	LEU	327	18.775	-8.688	23.891	1.00	31.26
	ATOM	154	C	LEU	327	20.156	-8.438	28.030	1.00	31.21
	ATOM	155	O	LEU	327	20.393	-7.578	28.891	1.00	30.12
60	ATOM	156	N	TYR	328	20.445	-9.725	28.181	1.00	30.99
	ATOM	157	CA	TYR	328	21.087	-10.229	29.381	1.00	30.95

5	ATOM	158	CB	TYR	328	20.409	-11.520	29.842	1.00	33.38
	ATOM	159	CG	TYR	328	19.194	-11.272	30.686	1.00	33.05
	ATOM	160	CD1	TYR	328	19.253	-11.398	32.071	1.00	31.92
	ATOM	161	CE1	TYR	328	18.152	-11.114	32.864	1.00	36.01
	ATOM	162	CD2	TYR	328	17.996	-10.862	30.110	1.00	36.05
10	ATOM	163	CE2	TYR	328	16.880	-10.574	30.899	1.00	37.27
	ATOM	164	CZ	TYR	328	16.973	-10.702	32.274	1.00	37.66
	ATOM	165	OH	TYR	328	15.896	-10.397	33.071	1.00	44.66
	ATOM	166	C	TYR	328	22.529	-10.520	29.067	1.00	33.66
	ATOM	167	O	TYR	328	22.884	-10.744	27.910	1.00	34.78
15	ATOM	168	N	SER	329	23.359	-10.496	30.103	1.00	33.97
	ATOM	169	CA	SER	329	24.767	-10.800	29.962	1.00	37.29
	ATOM	170	CB	SER	329	25.526	-10.342	31.204	1.00	36.51
	ATOM	171	OG	SER	329	26.787	-10.965	31.282	1.00	37.13
	ATOM	172	C	SER	329	24.835	-12.317	29.832	1.00	40.43
20	ATOM	173	O	SER	329	23.980	-13.028	30.363	1.00	40.11
	ATOM	174	N	GLU	330	25.845	-12.811	29.128	1.00	41.40
	ATOM	175	CA	GLU	330	25.992	-14.242	28.928	1.00	47.43
	ATOM	176	CB	GLU	330	26.423	-14.524	27.484	1.00	48.64
	ATOM	177	CG	GLU	330	25.278	-14.870	26.542	1.00	50.20
25	ATOM	178	CD	GLU	330	25.765	-15.405	25.198	1.00	53.25
	ATOM	179	OE1	GLU	330	25.909	-16.640	25.062	1.00	53.27
	ATOM	180	OE2	GLU	330	26.004	-14.590	24.280	1.00	51.80
	ATOM	181	C	GLU	330	26.999	-14.852	29.893	1.00	49.67
	ATOM	182	O	GLU	330	28.207	-14.741	29.696	1.00	50.11
30	ATOM	183	N	TYR	331	26.498	-15.493	30.942	1.00	53.62
	ATOM	184	CA	TYR	331	27.373	-16.130	31.921	1.00	58.16
	ATOM	185	CB	TYR	331	28.092	-15.078	32.774	1.00	59.55
	ATOM	186	CG	TYR	331	27.239	-14.460	33.860	1.00	63.08
	ATOM	187	CD1	TYR	331	26.656	-13.205	33.682	1.00	64.50
35	ATOM	188	CE1	TYR	331	25.864	-12.630	34.676	1.00	65.99
	ATOM	189	CD2	TYR	331	27.010	-15.128	35.065	1.00	63.52
	ATOM	190	CE2	TYR	331	26.219	-14.563	36.066	1.00	65.60
	ATOM	191	CZ	TYR	331	25.648	-13.314	35.864	1.00	67.20
	ATOM	192	OH	TYR	331	24.855	-12.753	36.839	1.00	67.40
40	ATOM	193	C	TYR	331	26.603	-17.080	32.823	1.00	59.05
	ATOM	194	O	TYR	331	25.393	-16.942	33.002	1.00	59.22
	ATOM	195	N	ASP	332	27.320	-18.045	33.387	1.00	61.62
	ATOM	196	CA	ASP	332	26.719	-19.026	34.281	1.00	64.20
	ATOM	197	CB	ASP	332	27.681	-20.194	34.500	1.00	65.99
45	ATOM	198	CG	ASP	332	26.961	-21.516	34.648	1.00	68.11
	ATOM	199	OD1	ASP	332	27.575	-22.564	34.351	1.00	69.54
	ATOM	200	OD2	ASP	332	25.781	-21.505	35.060	1.00	67.40
	ATOM	201	C	ASP	332	26.393	-18.371	35.619	1.00	63.33
	ATOM	202	O	ASP	332	27.292	-18.073	36.406	1.00	63.90
50	ATOM	203	N	PRO	333	25.096	-18.148	35.896	1.00	63.64
	ATOM	204	CD	PRO	333	23.945	-18.509	35.053	1.00	64.35
	ATOM	205	CA	PRO	333	24.677	-17.521	37.154	1.00	63.52
	ATOM	206	CB	PRO	333	23.165	-17.333	36.993	1.00	63.53
	ATOM	207	CG	PRO	333	22.866	-17.611	35.556	1.00	64.15
55	ATOM	208	C	PRO	333	25.010	-18.419	38.332	1.00	63.29
	ATOM	209	O	PRO	333	25.129	-17.964	39.468	1.00	63.28
	ATOM	210	N	THR	334	25.160	-19.704	38.037	1.00	64.26
	ATOM	211	CA	THR	334	25.475	-20.697	39.050	1.00	66.09
	ATOM	212	CB	THR	334	24.929	-22.080	38.645	1.00	66.90
60	ATOM	213	OG1	THR	334	25.571	-22.513	37.439	1.00	68.06
	ATOM	214	CG2	THR	334	23.423	-22.012	38.411	1.00	67.57

5	ATOM	215	C	THR	334	26.982	-20.804	39.269	1.00	65.67
	ATOM	216	O	THR	334	27.432	-21.323	40.289	1.00	64.77
	ATOM	217	N	ARG	335	27.759	-20.308	38.313	1.00	65.65
	ATOM	218	CA	ARG	335	29.214	-20.360	38.421	1.00	66.60
	ATOM	219	CB	ARG	335	29.835	-20.500	37.030	1.00	66.74
10	ATOM	220	C	ARG	335	29.757	-19.113	39.123	1.00	67.09
	ATOM	221	O	ARG	335	29.100	-18.071	39.148	1.00	67.31
	ATOM	222	N	PRO	336	30.968	-19.207	39.702	1.00	67.62
	ATOM	223	CD	PRO	336	31.820	-20.408	39.713	1.00	67.30
	ATOM	224	CA	PRO	336	31.601	-18.086	40.410	1.00	67.42
15	ATOM	225	CB	PRO	336	32.982	-18.621	40.783	1.00	66.43
	ATOM	226	CG	PRO	336	32.829	-20.097	40.779	1.00	67.52
	ATOM	227	C	PRO	336	31.701	-16.828	39.561	1.00	68.26
	ATOM	228	O	PRO	336	31.996	-16.895	38.371	1.00	69.04
	ATOM	229	N	PHE	337	31.460	-15.681	40.183	1.00	69.49
20	ATOM	230	CA	PHE	337	31.529	-14.408	39.480	1.00	71.39
	ATOM	231	CB	PHE	337	30.818	-13.323	40.294	1.00	72.31
	ATOM	232	CG	PHE	337	31.219	-11.924	39.921	1.00	73.21
	ATOM	233	CD1	PHE	337	30.632	-11.287	38.833	1.00	72.82
	ATOM	234	CD2	PHE	337	32.191	-11.245	40.653	1.00	73.43
25	ATOM	235	CE1	PHE	337	31.006	-9.993	38.479	1.00	73.28
	ATOM	236	CE2	PHE	337	32.573	-9.950	40.306	1.00	73.00
	ATOM	237	CZ	PHE	337	31.980	-9.323	39.217	1.00	72.90
	ATOM	238	C	PHE	337	32.985	-14.013	39.245	1.00	71.38
	ATOM	239	O	PHE	337	33.336	-13.487	38.189	1.00	71.56
30	ATOM	240	N	SER	338	33.825	-14.273	40.241	1.00	71.53
	ATOM	241	CA	SER	338	35.248	-13.947	40.172	1.00	70.98
	ATOM	242	CB	SER	338	35.957	-14.487	41.414	1.00	70.43
	ATOM	243	OG	SER	338	35.547	-15.818	41.679	1.00	69.59
	ATOM	244	C	SER	338	35.931	-14.504	38.924	1.00	71.20
35	ATOM	245	O	SER	338	36.951	-13.972	38.475	1.00	71.35
	ATOM	246	N	GLU	339	35.368	-15.573	38.369	1.00	70.20
	ATOM	247	CA	GLU	339	35.930	-16.215	37.183	1.00	69.48
	ATOM	248	CB	GLU	339	35.279	-17.585	36.971	1.00	71.07
	ATOM	249	CG	GLU	339	35.996	-18.740	37.656	1.00	72.60
40	ATOM	250	CD	GLU	339	35.382	-20.089	37.318	1.00	74.26
	ATOM	251	OE1	GLU	339	34.786	-20.220	36.227	1.00	73.51
	ATOM	252	OE2	GLU	339	35.496	-21.020	38.144	1.00	76.44
	ATOM	253	C	GLU	339	35.770	-15.385	35.910	1.00	68.15
	ATOM	254	O	GLU	339	36.722	-15.216	35.144	1.00	68.99
45	ATOM	255	N	ALA	340	34.562	-14.874	35.694	1.00	64.41
	ATOM	256	CA	ALA	340	34.246	-14.083	34.507	1.00	60.69
	ATOM	257	CB	ALA	340	32.767	-13.709	34.523	1.00	61.17
	ATOM	258	C	ALA	340	35.096	-12.824	34.326	1.00	57.00
	ATOM	259	O	ALA	340	35.634	-12.270	35.287	1.00	57.46
50	ATOM	260	N	SER	341	35.215	-12.388	33.076	1.00	52.15
	ATOM	261	CA	SER	341	35.972	-11.188	32.736	1.00	46.53
	ATOM	262	CB	SER	341	36.839	-11.439	31.497	1.00	48.64
	ATOM	263	OG	SER	341	37.184	-10.226	30.846	1.00	46.48
	ATOM	264	C	SER	341	34.957	-10.087	32.444	1.00	43.52
55	ATOM	265	O	SER	341	34.090	-10.248	31.589	1.00	39.92
	ATOM	266	N	MET	342	35.052	-8.978	33.166	1.00	41.24
	ATOM	267	CA	MET	342	34.121	-7.875	32.960	1.00	42.46
	ATOM	268	CB	MET	342	34.449	-6.723	33.912	1.00	45.61
	ATOM	269	CG	MET	342	33.228	-6.089	34.560	1.00	52.39
60	ATOM	270	SD	MET	342	31.791	-7.201	34.631	1.00	57.92
	ATOM	271	CE	MET	342	31.999	-7.881	36.239	1.00	56.18

5	ATOM	272	C	MET	342	34.124	-7.365	31.516	1.00	40.22
	ATOM	273	O	MET	342	33.063	-7.121	30.938	1.00	39.23
	ATOM	274	N	MET	343	35.307	-7.204	30.930	1.00	38.72
	ATOM	275	CA	MET	343	35.395	-6.708	29.558	1.00	38.50
	ATOM	276	CB	MET	343	36.838	-6.318	29.216	1.00	41.15
10	ATOM	277	CG	MET	343	37.022	-5.749	27.804	1.00	40.31
	ATOM	278	SD	MET	343	36.032	-4.260	27.427	1.00	45.23
	ATOM	279	CE	MET	343	36.113	-3.358	28.987	1.00	40.45
	ATOM	280	C	MET	343	34.880	-7.741	28.561	1.00	35.36
	ATOM	281	O	MET	343	34.368	-7.384	27.501	1.00	35.51
15	ATOM	282	N	GLY	344	35.017	-9.020	28.902	1.00	35.53
	ATOM	283	CA	GLY	344	34.533	-10.072	28.024	1.00	33.41
	ATOM	284	C	GLY	344	33.015	-10.063	28.047	1.00	31.74
	ATOM	285	O	GLY	344	32.359	-10.233	27.019	1.00	29.58
	ATOM	286	N	LEU	345	32.459	-9.860	29.238	1.00	32.89
20	ATOM	287	CA	LEU	345	31.011	-9.804	29.415	1.00	34.95
	ATOM	288	CB	LEU	345	30.665	-9.631	30.902	1.00	37.56
	ATOM	289	CG	LEU	345	30.942	-10.774	31.883	1.00	43.03
	ATOM	290	CD1	LEU	345	30.537	-10.357	33.297	1.00	41.57
	ATOM	291	CD2	LEU	345	30.164	-11.998	31.449	1.00	42.80
25	ATOM	292	C	LEU	345	30.430	-8.614	28.633	1.00	33.71
	ATOM	293	O	LEU	345	29.479	-8.757	27.868	1.00	30.29
	ATOM	294	N	LEU	346	31.021	-7.443	28.843	1.00	30.20
	ATOM	295	CA	LEU	346	30.569	-6.217	28.193	1.00	32.00
	ATOM	296	CB	LEU	346	31.317	-5.016	28.771	1.00	28.16
30	ATOM	297	CG	LEU	346	31.091	-4.767	30.269	1.00	29.84
	ATOM	298	CD1	LEU	346	31.815	-3.498	30.668	1.00	29.98
	ATOM	299	CD2	LEU	346	29.614	-4.644	30.581	1.00	33.97
	ATOM	300	C	LEU	346	30.732	-6.250	26.682	1.00	30.70
	ATOM	301	O	LEU	346	29.869	-5.765	25.955	1.00	29.13
35	ATOM	302	N	THR	347	31.839	-6.816	26.212	1.00	30.47
	ATOM	303	CA	THR	347	32.086	-6.911	24.781	1.00	30.93
	ATOM	304	CB	THR	347	33.472	-7.501	24.497	1.00	29.97
	ATOM	305	OG1	THR	347	34.481	-6.604	24.982	1.00	35.40
	ATOM	306	CG2	THR	347	33.666	-7.707	23.004	1.00	33.58
40	ATOM	307	C	THR	347	31.036	-7.804	24.122	1.00	31.97
	ATOM	308	O	THR	347	30.516	-7.486	23.049	1.00	30.75
	ATOM	309	N	ASN	348	30.737	-8.926	24.768	1.00	29.31
	ATOM	310	CA	ASN	348	29.757	-9.868	24.242	1.00	32.63
	ATOM	311	CB	ASN	348	29.767	-11.161	25.065	1.00	31.64
45	ATOM	312	CG	ASN	348	28.646	-12.117	24.662	1.00	39.14
	ATOM	313	OD1	ASN	348	27.549	-12.078	25.220	1.00	41.91
	ATOM	314	ND2	ASN	348	28.920	-12.970	23.683	1.00	42.05
	ATOM	315	C	ASN	348	28.361	-9.251	24.262	1.00	29.02
	ATOM	316	O	ASN	348	27.558	-9.477	23.353	1.00	32.76
50	ATOM	317	N	LEU	349	28.078	-8.467	25.298	1.00	28.74
	ATOM	318	CA	LEU	349	26.782	-7.811	25.421	1.00	28.58
	ATOM	319	CB	LEU	349	26.650	-7.148	26.795	1.00	26.56
	ATOM	320	CG	LEU	349	25.376	-6.328	27.050	1.00	33.67
	ATOM	321	CD1	LEU	349	24.140	-7.199	26.840	1.00	28.82
55	ATOM	322	CD2	LEU	349	25.392	-5.779	28.471	1.00	33.11
	ATOM	323	C	LEU	349	26.638	-6.762	24.319	1.00	28.07
	ATOM	324	O	LEU	349	25.616	-6.703	23.629	1.00	25.22
	ATOM	325	N	ALA	350	27.675	-5.941	24.157	1.00	28.50
	ATOM	326	CA	ALA	350	27.668	-4.886	23.148	1.00	28.46
60	ATOM	327	CB	ALA	350	28.972	-4.094	23.209	1.00	28.12
	ATOM	328	C	ALA	350	27.468	-5.461	21.750	1.00	28.75

5	ATOM	329	O	ALA	350	26.649	-4.958	20.983	1.00	30.90
	ATOM	330	N	ASP	351	28.213	-6.509	21.420	1.00	27.20
	ATOM	331	CA	ASP	351	28.093	-7.143	20.112	1.00	29.75
	ATOM	332	CB	ASP	351	29.036	-8.345	20.010	1.00	34.16
	ATOM	333	CG	ASP	351	30.498	-7.940	19.978	1.00	37.50
10	ATOM	334	OD1	ASP	351	31.354	-8.831	20.148	1.00	37.55
	ATOM	335	OD2	ASP	351	30.789	-6.738	19.784	1.00	35.50
	ATOM	336	C	ASP	351	26.661	-7.600	19.813	1.00	30.52
	ATOM	337	O	ASP	351	26.193	-7.458	18.687	1.00	27.77
	ATOM	338	N	ARG	352	25.968	-8.150	20.811	1.00	27.18
15	ATOM	339	CA	ARG	352	24.593	-8.602	20.605	1.00	26.21
	ATOM	340	CB	ARG	352	24.148	-9.534	21.752	1.00	26.52
	ATOM	341	CG	ARG	352	24.567	-10.991	21.532	1.00	31.03
	ATOM	342	CD	ARG	352	24.128	-11.911	22.666	1.00	29.80
	ATOM	343	NE	ARG	352	24.898	-11.675	23.879	1.00	30.44
20	ATOM	344	CZ	ARG	352	24.364	-11.363	25.054	1.00	31.68
	ATOM	345	NH1	ARG	352	23.050	-11.251	25.177	1.00	31.18
	ATOM	346	NH2	ARG	352	25.144	-11.148	26.104	1.00	32.03
	ATOM	347	C	ARG	352	23.642	-7.411	20.502	1.00	27.16
	ATOM	348	O	ARG	352	22.702	-7.426	19.708	1.00	26.65
25	ATOM	349	N	GLU	353	23.896	-6.370	21.291	1.00	24.30
	ATOM	350	CA	GLU	353	23.045	-5.178	21.261	1.00	26.39
	ATOM	351	CB	GLU	353	23.461	-4.204	22.365	1.00	24.91
	ATOM	352	CG	GLU	353	23.147	-4.669	23.771	1.00	27.93
	ATOM	353	CD	GLU	353	23.425	-3.587	24.795	1.00	30.71
30	ATOM	354	OE1	GLU	353	24.564	-3.534	25.304	1.00	30.09
	ATOM	355	OE2	GLU	353	22.506	-2.789	25.085	1.00	30.53
	ATOM	356	C	GLU	353	23.131	-4.456	19.920	1.00	24.27
	ATOM	357	O	GLU	353	22.169	-3.826	19.467	1.00	28.71
	ATOM	358	N	LEU	354	24.296	-4.540	19.293	1.00	26.61
35	ATOM	359	CA	LEU	354	24.522	-3.872	18.017	1.00	26.62
	ATOM	360	CB	LEU	354	25.952	-4.121	17.543	1.00	26.36
	ATOM	361	CG	LEU	354	26.372	-3.257	16.351	1.00	29.24
	ATOM	362	CD1	LEU	354	26.243	-1.774	16.722	1.00	26.59
	ATOM	363	CD2	LEU	354	27.794	-3.607	15.962	1.00	28.88
40	ATOM	364	C	LEU	354	23.559	-4.300	16.926	1.00	27.72
	ATOM	365	O	LEU	354	23.074	-3.475	16.152	1.00	24.00
	ATOM	366	N	VAL	355	23.291	-5.598	16.854	1.00	28.82
	ATOM	367	CA	VAL	355	22.386	-6.125	15.844	1.00	29.45
	ATOM	368	CB	VAL	355	22.259	-7.655	15.975	1.00	31.76
45	ATOM	369	CG1	VAL	355	21.423	-8.205	14.834	1.00	33.55
	ATOM	370	CG2	VAL	355	23.649	-8.282	15.998	1.00	31.36
	ATOM	371	C	VAL	355	21.020	-5.499	16.035	1.00	27.71
	ATOM	372	O	VAL	355	20.382	-5.039	15.080	1.00	29.61
	ATOM	373	N	HIS	356	20.580	-5.473	17.288	1.00	27.76
50	ATOM	374	CA	HIS	356	19.291	-4.906	17.627	1.00	28.35
	ATOM	375	CB	HIS	356	18.936	-5.231	19.079	1.00	31.12
	ATOM	376	CG	HIS	356	18.602	-6.675	19.307	1.00	35.93
	ATOM	377	CD2	HIS	356	19.352	-7.700	19.779	1.00	33.95
	ATOM	378	ND1	HIS	356	17.363	-7.208	19.018	1.00	36.62
55	ATOM	379	CE1	HIS	356	17.364	-8.499	19.304	1.00	33.33
	ATOM	380	NE2	HIS	356	18.559	-8.823	19.767	1.00	32.16
	ATOM	381	C	HIS	356	19.300	-3.398	17.412	1.00	28.25
	ATOM	382	O	HIS	356	18.272	-2.812	17.100	1.00	28.99
	ATOM	383	N	MET	357	20.457	-2.765	17.574	1.00	25.31
60	ATOM	384	CA	MET	357	20.526	-1.322	17.369	1.00	24.63
	ATOM	385	CB	MET	357	21.902	-0.789	17.766	1.00	23.61



5	ATOM	386	CG	MET	357	22.011	0.736	17.699	1.00	24.66
	ATOM	387	SD	MET	357	23.732	1.290	17.859	1.00	27.30
	ATOM	388	CE	MET	357	24.140	0.672	19.514	1.00	23.62
	ATOM	389	C	MET	357	20.256	-1.011	15.898	1.00	24.83
	ATOM	390	O	MET	357	19.619	-0.003	15.569	1.00	26.78
10	ATOM	391	N	ILE	358	20.757	-1.874	15.020	1.00	26.25
	ATOM	392	CA	ILE	358	20.553	-1.721	13.576	1.00	30.33
	ATOM	393	CB	ILE	358	21.204	-2.888	12.789	1.00	33.86
	ATOM	394	CG2	ILE	358	20.759	-2.860	11.334	1.00	33.68
	ATOM	395	CG1	ILE	358	22.728	-2.799	12.874	1.00	36.89
15	ATOM	396	CD1	ILE	358	23.299	-1.469	12.451	1.00	39.10
	ATOM	397	C	ILE	358	19.055	-1.721	13.310	1.00	32.20
	ATOM	398	O	ILE	358	18.519	-0.817	12.662	1.00	32.02
	ATOM	399	N	ASN	359	18.379	-2.748	13.814	1.00	33.12
	ATOM	400	CA	ASN	359	16.945	-2.861	13.638	1.00	33.35
20	ATOM	401	CB	ASN	359	16.434	-4.101	14.363	1.00	37.59
	ATOM	402	CG	ASN	359	16.739	-5.374	13.627	1.00	44.38
	ATOM	403	OD1	ASN	359	17.045	-5.329	12.437	1.00	47.35
	ATOM	404	ND2	ASN	359	16.673	-6.508	14.320	1.00	42.48
	ATOM	405	C	ASN	359	16.224	-1.634	14.149	1.00	32.74
25	ATOM	406	O	ASN	359	15.261	-1.163	13.530	1.00	31.39
	ATOM	407	N	TRP	360	16.706	-1.104	15.264	1.00	27.92
	ATOM	408	CA	TRP	360	16.102	0.087	15.842	1.00	29.47
	ATOM	409	CB	TRP	360	16.703	0.347	17.228	1.00	27.66
	ATOM	410	CG	TRP	360	16.522	1.747	17.707	1.00	30.40
30	ATOM	411	CD2	TRP	360	17.493	2.801	17.657	1.00	27.54
	ATOM	412	CE2	TRP	360	16.888	3.954	18.204	1.00	29.42
	ATOM	413	CE3	TRP	360	18.819	2.883	17.205	1.00	28.37
	ATOM	414	CD1	TRP	360	15.399	2.284	18.264	1.00	27.75
	ATOM	415	NE1	TRP	360	15.609	3.611	18.566	1.00	30.84
35	ATOM	416	CZ2	TRP	360	17.558	5.180	18.310	1.00	27.74
	ATOM	417	CZ3	TRP	360	19.488	4.106	17.309	1.00	24.49
	ATOM	418	CH2	TRP	360	18.853	5.232	17.858	1.00	25.09
	ATOM	419	C	TRP	360	16.312	1.296	14.926	1.00	27.90
	ATOM	420	O	TRP	360	15.360	2.002	14.581	1.00	28.83
40	ATOM	421	N	ALA	361	17.559	1.520	14.523	1.00	28.25
	ATOM	422	CA	ALA	361	17.894	2.637	13.645	1.00	29.20
	ATOM	423	CB	ALA	361	19.346	2.539	13.220	1.00	28.89
	ATOM	424	C	ALA	361	17.006	2.685	12.403	1.00	31.08
	ATOM	425	O	ALA	361	16.531	3.746	12.011	1.00	31.30
45	ATOM	426	N	LYS	362	16.795	1.526	11.783	1.00	30.93
	ATOM	427	CA	LYS	362	15.981	1.443	10.581	1.00	34.15
	ATOM	428	CB	LYS	362	16.012	0.016	10.023	1.00	33.67
	ATOM	429	CG	LYS	362	17.252	-0.281	9.198	1.00	39.40
	ATOM	430	CD	LYS	362	17.547	-1.774	9.136	1.00	43.60
50	ATOM	431	CE	LYS	362	18.852	-2.046	8.389	1.00	47.06
	ATOM	432	NZ	LYS	362	19.178	-3.507	8.288	1.00	50.34
	ATOM	433	C	LYS	362	14.545	1.872	10.815	1.00	35.81
	ATOM	434	O	LYS	362	13.821	2.168	9.859	1.00	37.95
	ATOM	435	N	ARG	363	14.134	1.921	12.079	1.00	34.23
55	ATOM	436	CA	ARG	363	12.770	2.313	12.409	1.00	36.04
	ATOM	437	CB	ARG	363	12.178	1.307	13.391	1.00	36.71
	ATOM	438	CG	ARG	363	12.169	-0.110	12.827	1.00	40.36
	ATOM	439	CD	ARG	363	11.468	-1.086	13.746	1.00	42.17
	ATOM	440	NE	ARG	363	10.161	-0.586	14.158	1.00	45.19
60	ATOM	441	CZ	ARG	363	9.314	-1.262	14.929	1.00	49.41
	ATOM	442	NH1	ARG	363	9.642	-2.467	15.374	1.00	48.02

5	ATOM	443	NH2	ARG	363	8.143	-0.729	15.261	1.00	51.54
	ATOM	444	C	ARG	363	12.654	3.743	12.943	1.00	37.40
	ATOM	445	O	ARG	363	11.567	4.199	13.303	1.00	38.22
	ATOM	446	N	VAL	364	13.785	4.442	13.002	1.00	35.66
	ATOM	447	CA	VAL	364	13.804	5.836	13.431	1.00	34.06
10	ATOM	448	CB	VAL	364	15.231	6.271	13.827	1.00	33.87
	ATOM	449	CG1	VAL	364	15.293	7.779	13.995	1.00	31.08
	ATOM	450	CG2	VAL	364	15.641	5.571	15.113	1.00	31.30
	ATOM	451	C	VAL	364	13.360	6.591	12.171	1.00	33.19
	ATOM	452	O	VAL	364	14.028	6.531	11.146	1.00	33.04
15	ATOM	453	N	PRO	365	12.225	7.310	12.234	1.00	34.69
	ATOM	454	CD	PRO	365	11.359	7.492	13.413	1.00	34.19
	ATOM	455	CA	PRO	365	11.724	8.050	11.069	1.00	35.96
	ATOM	456	CB	PRO	365	10.608	8.918	11.645	1.00	36.59
	ATOM	457	CG	PRO	365	10.135	8.157	12.842	1.00	39.59
20	ATOM	458	C	PRO	365	12.756	8.878	10.321	1.00	37.19
	ATOM	459	O	PRO	365	13.430	9.726	10.907	1.00	40.29
	ATOM	460	N	GLY	366	12.878	8.624	9.023	1.00	34.78
	ATOM	461	CA	GLY	366	13.816	9.371	8.212	1.00	33.54
	ATOM	462	C	GLY	366	15.168	8.722	8.007	1.00	34.26
25	ATOM	463	O	GLY	366	15.858	9.035	7.034	1.00	37.15
	ATOM	464	N	PHE	367	15.554	7.814	8.901	1.00	33.13
	ATOM	465	CA	PHE	367	16.860	7.164	8.787	1.00	32.04
	ATOM	466	CB	PHE	367	17.138	6.291	10.016	1.00	30.22
	ATOM	467	CG	PHE	367	18.544	5.773	10.080	1.00	30.60
30	ATOM	468	CD1	PHE	367	18.827	4.446	9.751	1.00	31.94
	ATOM	469	CD2	PHE	367	19.589	6.601	10.485	1.00	29.20
	ATOM	470	CE1	PHE	367	20.133	3.950	9.828	1.00	28.30
	ATOM	471	CE2	PHE	367	20.896	6.122	10.568	1.00	28.12
	ATOM	472	CZ	PHE	367	21.171	4.791	10.240	1.00	25.41
35	ATOM	473	C	PHE	367	17.033	6.333	7.524	1.00	31.46
	ATOM	474	O	PHE	367	18.073	6.405	6.883	1.00	32.30
	ATOM	475	N	VAL	368	16.027	5.541	7.165	1.00	35.20
	ATOM	476	CA	VAL	368	16.123	4.718	5.959	1.00	38.98
	ATOM	477	CB	VAL	368	15.076	3.584	5.945	1.00	40.61
40	ATOM	478	CG1	VAL	368	15.543	2.447	6.843	1.00	41.48
	ATOM	479	CG2	VAL	368	13.717	4.113	6.390	1.00	41.60
	ATOM	480	C	VAL	368	15.965	5.523	4.673	1.00	40.06
	ATOM	481	O	VAL	368	16.156	4.992	3.579	1.00	41.66
	ATOM	482	N	ASP	369	15.608	6.798	4.798	1.00	38.65
45	ATOM	483	CA	ASP	369	15.465	7.646	3.621	1.00	37.15
	ATOM	484	CB	ASP	369	14.700	8.929	3.954	1.00	39.89
	ATOM	485	CG	ASP	369	13.254	8.671	4.302	1.00	45.59
	ATOM	486	OD1	ASP	369	12.686	7.672	3.806	1.00	46.34
	ATOM	487	OD2	ASP	369	12.681	9.472	5.074	1.00	49.13
50	ATOM	488	C	ASP	369	16.855	8.010	3.136	1.00	34.91
	ATOM	489	O	ASP	369	17.038	8.431	1.995	1.00	34.25
	ATOM	490	N	LEU	370	17.838	7.841	4.016	1.00	31.76
	ATOM	491	CA	LEU	370	19.229	8.153	3.705	1.00	28.08
	ATOM	492	CB	LEU	370	20.020	8.339	5.003	1.00	28.81
55	ATOM	493	CG	LEU	370	19.523	9.395	6.000	1.00	28.74
	ATOM	494	CD1	LEU	370	20.315	9.275	7.299	1.00	30.81
	ATOM	495	CD2	LEU	370	19.693	10.792	5.404	1.00	29.77
	ATOM	496	C	LEU	370	19.884	7.043	2.893	1.00	31.25
	ATOM	497	O	LEU	370	19.341	5.943	2.784	1.00	31.78
60	ATOM	498	N	THR	371	21.052	7.333	2.331	1.00	28.86
	ATOM	499	CA	THR	371	21.793	6.336	1.569	1.00	32.90

5	ATOM	500	CB	THR	371	22.979	6.944	0.818	1.00	33.44
	ATOM	501	OG1	THR	371	23.880	7.523	1.766	1.00	34.59
	ATOM	502	CG2	THR	371	22.514	8.002	-0.178	1.00	32.63
	ATOM	503	C	THR	371	22.373	5.315	2.539	1.00	35.31
	ATOM	504	O	THR	371	22.536	5.591	3.733	1.00	31.27
10	ATOM	505	N	LEU	372	22.702	4.141	2.015	1.00	34.34
	ATOM	506	CA	LEU	372	23.273	3.073	2.822	1.00	35.46
	ATOM	507	CB	LEU	372	23.518	1.841	1.944	1.00	37.73
	ATOM	508	CG	LEU	372	24.362	0.704	2.515	1.00	42.43
	ATOM	509	CD1	LEU	372	23.690	0.145	3.757	1.00	45.60
15	ATOM	510	CD2	LEU	372	24.534	-0.383	1.455	1.00	44.29
	ATOM	511	C	LEU	372	24.587	3.548	3.444	1.00	36.95
	ATOM	512	O	LEU	372	24.813	3.374	4.643	1.00	35.57
	ATOM	513	N	HIS	373	25.442	4.159	2.627	1.00	35.68
	ATOM	514	CA	HIS	373	26.729	4.656	3.099	1.00	36.60
20	ATOM	515	CB	HIS	373	27.506	5.282	1.935	1.00	44.01
	ATOM	516	CG	HIS	373	28.538	6.280	2.360	1.00	50.69
	ATOM	517	CD2	HIS	373	29.857	6.138	2.636	1.00	54.69
	ATOM	518	ND1	HIS	373	28.246	7.613	2.561	1.00	53.77
	ATOM	519	CE1	HIS	373	29.339	8.248	2.945	1.00	57.09
25	ATOM	520	NE2	HIS	373	30.331	7.376	2.999	1.00	57.23
	ATOM	521	C	HIS	373	26.575	5.669	4.244	1.00	36.22
	ATOM	522	O	HIS	373	27.350	5.650	5.201	1.00	33.05
	ATOM	523	N	ASP	374	25.580	6.549	4.148	1.00	32.03
	ATOM	524	CA	ASP	374	25.342	7.541	5.196	1.00	30.76
30	ATOM	525	CB	ASP	374	24.354	8.603	4.713	1.00	30.12
	ATOM	526	CG	ASP	374	25.018	9.672	3.860	1.00	35.83
	ATOM	527	OD1	ASP	374	26.264	9.744	3.842	1.00	34.39
	ATOM	528	OD2	ASP	374	24.291	10.440	3.199	1.00	35.39
	ATOM	529	C	ASP	374	24.805	6.876	6.472	1.00	30.33
35	ATOM	530	O	ASP	374	25.152	7.275	7.587	1.00	27.04
	ATOM	531	N	GLN	375	23.944	5.877	6.309	1.00	25.71
	ATOM	532	CA	GLN	375	23.403	5.157	7.454	1.00	26.68
	ATOM	533	CB	GLN	375	22.424	4.077	6.993	1.00	29.70
	ATOM	534	CG	GLN	375	21.101	4.616	6.484	1.00	29.16
40	ATOM	535	CD	GLN	375	20.219	3.514	5.940	1.00	35.87
	ATOM	536	OE1	GLN	375	20.155	2.426	6.510	1.00	30.97
	ATOM	537	NE2	GLN	375	19.541	3.785	4.827	1.00	34.51
	ATOM	538	C	GLN	375	24.556	4.502	8.214	1.00	25.51
	ATOM	539	O	GLN	375	24.585	4.513	9.442	1.00	28.14
45	ATOM	540	N	VAL	376	25.504	3.938	7.475	1.00	26.62
	ATOM	541	CA	VAL	376	26.659	3.281	8.071	1.00	29.24
	ATOM	542	CB	VAL	376	27.531	2.597	7.003	1.00	29.66
	ATOM	543	CG1	VAL	376	28.812	2.071	7.635	1.00	28.29
	ATOM	544	CG2	VAL	376	26.745	1.469	6.341	1.00	29.90
50	ATOM	545	C	VAL	376	27.526	4.285	8.821	1.00	30.87
	ATOM	546	O	VAL	376	27.953	4.029	9.948	1.00	30.09
	ATOM	547	N	HIS	377	27.785	5.428	8.191	1.00	28.05
	ATOM	548	CA	HIS	377	28.602	6.457	8.814	1.00	28.68
	ATOM	549	CB	HIS	377	28.792	7.639	7.864	1.00	30.26
55	ATOM	550	CG	HIS	377	29.508	8.791	8.488	1.00	33.89
	ATOM	551	CD2	HIS	377	29.073	10.017	8.863	1.00	34.99
	ATOM	552	ND1	HIS	377	30.846	8.740	8.823	1.00	37.01
	ATOM	553	CE1	HIS	377	31.201	9.884	9.377	1.00	34.79
	ATOM	554	NE2	HIS	377	30.144	10.677	9.413	1.00	34.95
60	ATOM	555	C	HIS	377	27.983	6.954	10.114	1.00	25.13
	ATOM	556	O	HIS	377	28.677	7.102	11.115	1.00	25.93

5	ATOM	557	N	LEU	378	26.678	7.206	10.107	1.00	24.58
	ATOM	558	CA	LEU	378	26.015	7.695	11.315	1.00	26.40
	ATOM	559	CB	LEU	378	24.542	8.001	11.027	1.00	26.29
	ATOM	560	CG	LEU	378	24.291	9.180	10.073	1.00	28.06
	ATOM	561	CD1	LEU	378	22.778	9.353	9.869	1.00	27.66
10	ATOM	562	CD2	LEU	378	24.911	10.458	10.642	1.00	30.08
	ATOM	563	C	LEU	378	26.120	6.695	12.459	1.00	28.55
	ATOM	564	O	LEU	378	26.379	7.075	13.605	1.00	24.76
	ATOM	565	N	LEU	379	25.919	5.414	12.153	1.00	24.29
	ATOM	566	CA	LEU	379	26.000	4.388	13.182	1.00	27.03
15	ATOM	567	CB	LEU	379	25.401	3.073	12.667	1.00	28.53
	ATOM	568	CG	LEU	379	23.875	3.023	12.845	1.00	30.29
	ATOM	569	CD1	LEU	379	23.248	1.943	11.963	1.00	33.04
	ATOM	570	CD2	LEU	379	23.563	2.759	14.312	1.00	29.45
	ATOM	571	C	LEU	379	27.430	4.176	13.670	1.00	27.18
20	ATOM	572	O	LEU	379	27.653	3.979	14.866	1.00	25.95
	ATOM	573	N	GLU	380	28.402	4.236	12.762	1.00	25.86
	ATOM	574	CA	GLU	380	29.786	4.054	13.173	1.00	27.58
	ATOM	575	CB	GLU	380	30.730	4.036	11.968	1.00	30.36
	ATOM	576	CG	GLU	380	32.172	3.785	12.380	1.00	37.98
25	ATOM	577	CD	GLU	380	33.080	3.471	11.210	1.00	45.23
	ATOM	578	OE1	GLU	380	32.869	4.048	10.120	1.00	42.99
	ATOM	579	OE2	GLU	380	34.004	2.646	11.386	1.00	45.79
	ATOM	580	C	GLU	380	30.218	5.159	14.133	1.00	27.50
	ATOM	581	O	GLU	380	31.056	4.937	15.010	1.00	26.67
30	ATOM	582	N	ACYS	381	29.637	6.339	13.965	0.75	24.89
	ATOM	583	N	BCYS	381	29.645	6.352	13.980	0.25	25.79
	ATOM	584	CA	ACYS	381	29.969	7.466	14.826	0.75	24.12
	ATOM	585	CA	BCYS	381	29.993	7.481	14.847	0.25	24.86
	ATOM	586	CB	ACYS	381	29.621	8.781	14.122	0.75	25.96
35	ATOM	587	CB	BCYS	381	29.766	8.814	14.115	0.25	25.62
	ATOM	588	SG	ACYS	381	30.698	9.192	12.732	0.75	31.63
	ATOM	589	SG	BCYS	381	30.227	10.312	15.059	0.25	25.40
	ATOM	590	C	ACYS	381	29.237	7.422	16.162	0.75	22.07
	ATOM	591	C	BCYS	381	29.211	7.498	16.159	0.25	23.97
40	ATOM	592	O	ACYS	381	29.812	7.730	17.206	0.75	21.97
	ATOM	593	O	BCYS	381	29.724	7.940	17.187	0.25	23.99
	ATOM	594	N	ALA	382	27.974	7.012	16.128	1.00	23.41
	ATOM	595	CA	ALA	382	27.140	7.015	17.318	1.00	22.83
	ATOM	596	CB	ALA	382	25.785	7.587	16.948	1.00	25.50
45	ATOM	597	C	ALA	382	26.913	5.755	18.131	1.00	25.39
	ATOM	598	O	ALA	382	26.374	5.837	19.234	1.00	23.09
	ATOM	599	N	TRP	383	27.311	4.602	17.615	1.00	25.98
	ATOM	600	CA	TRP	383	27.026	3.354	18.318	1.00	23.80
	ATOM	601	CB	TRP	383	27.669	2.172	17.580	1.00	22.52
50	ATOM	602	CG	TRP	383	29.130	2.054	17.762	1.00	24.42
	ATOM	603	CD2	TRP	383	29.797	1.347	18.803	1.00	27.31
	ATOM	604	CE2	TRP	383	31.182	1.484	18.579	1.00	28.24
	ATOM	605	CE3	TRP	383	29.360	0.609	19.912	1.00	27.37
	ATOM	606	CD1	TRP	383	30.102	2.578	16.965	1.00	24.58
55	ATOM	607	NE1	TRP	383	31.342	2.239	17.446	1.00	27.35
	ATOM	608	CZ2	TRP	383	32.133	0.909	19.420	1.00	28.76
	ATOM	609	CZ3	TRP	383	30.305	0.039	20.745	1.00	28.09
	ATOM	610	CH2	TRP	383	31.674	0.191	20.496	1.00	29.77
	ATOM	611	C	TRP	383	27.356	3.309	19.802	1.00	23.54
60	ATOM	612	O	TRP	383	26.526	2.866	20.584	1.00	22.90
	ATOM	613	N	LEU	384	28.542	3.765	20.211	1.00	20.37

5	ATOM	614	CA	LEU	384	28.864	3.713	21.640	1.00	22.41
	ATOM	615	CB	LEU	384	30.369	3.890	21.883	1.00	24.98
	ATOM	616	CG	LEU	384	30.824	3.645	23.336	1.00	27.33
	ATOM	617	CD1	LEU	384	30.273	2.305	23.853	1.00	29.71
10	ATOM	618	CD2	LEU	384	32.336	3.648	23.398	1.00	26.07
	ATOM	619	C	LEU	384	28.075	4.732	22.453	1.00	19.44
	ATOM	620	O	LEU	384	27.706	4.458	23.595	1.00	23.24
	ATOM	621	N	GLU	385	27.807	5.909	21.885	1.00	20.80
15	ATOM	622	CA	GLU	385	27.011	6.895	22.612	1.00	21.32
	ATOM	623	CB	GLU	385	26.861	8.177	21.797	1.00	21.91
	ATOM	624	CG	GLU	385	28.115	9.020	21.705	1.00	21.61
	ATOM	625	CD	GLU	385	27.882	10.256	20.860	1.00	29.53
20	ATOM	626	OE1	GLU	385	27.374	11.256	21.401	1.00	30.54
	ATOM	627	OE2	GLU	385	28.188	10.219	19.658	1.00	29.97
	ATOM	628	C	GLU	385	25.616	6.292	22.836	1.00	22.26
	ATOM	629	O	GLU	385	25.022	6.438	23.902	1.00	22.26
25	ATOM	630	N	ILE	386	25.101	5.617	21.812	1.00	22.03
	ATOM	631	CA	ILE	386	23.779	4.995	21.896	1.00	22.74
	ATOM	632	CB	ILE	386	23.328	4.455	20.498	1.00	22.88
	ATOM	633	CG2	ILE	386	22.009	3.647	20.618	1.00	23.85
30	ATOM	634	CG1	ILE	386	23.085	5.651	19.561	1.00	25.05
	ATOM	635	CD1	ILE	386	22.994	5.297	18.078	1.00	26.42
	ATOM	636	C	ILE	386	23.766	3.897	22.961	1.00	22.50
	ATOM	637	O	ILE	386	22.823	3.818	23.746	1.00	24.75
35	ATOM	638	N	LEU	387	24.810	3.071	23.020	1.00	22.25
	ATOM	639	CA	LEU	387	24.868	2.030	24.051	1.00	22.95
	ATOM	640	CB	LEU	387	26.096	1.132	23.864	1.00	24.61
	ATOM	641	CG	LEU	387	26.070	0.194	22.654	1.00	23.21
40	ATOM	642	CD1	LEU	387	27.297	-0.709	22.705	1.00	25.36
	ATOM	643	CD2	LEU	387	24.791	-0.631	22.652	1.00	26.29
	ATOM	644	C	LEU	387	24.944	2.660	25.438	1.00	26.22
	ATOM	645	O	LEU	387	24.287	2.204	26.386	1.00	23.55
45	ATOM	646	N	MET	388	25.751	3.713	25.554	1.00	23.92
	ATOM	647	CA	MET	388	25.924	4.385	26.835	1.00	24.26
	ATOM	648	CB	MET	388	27.088	5.378	26.761	1.00	23.87
	ATOM	649	CG	MET	388	28.440	4.722	26.743	1.00	24.08
50	ATOM	650	SD	MET	388	29.726	5.992	26.736	1.00	27.70
	ATOM	651	CE	MET	388	31.139	5.041	27.078	1.00	21.74
	ATOM	652	C	MET	388	24.660	5.094	27.321	1.00	23.33
	ATOM	653	O	MET	388	24.341	5.026	28.505	1.00	25.58
55	ATOM	654	N	ILE	389	23.935	5.775	26.436	1.00	24.62
	ATOM	655	CA	ILE	389	22.729	6.440	26.905	1.00	24.03
	ATOM	656	CB	ILE	389	22.132	7.439	25.852	1.00	27.01
	ATOM	657	CG2	ILE	389	21.413	6.705	24.706	1.00	23.98
60	ATOM	658	CG1	ILE	389	21.185	8.402	26.584	1.00	25.49
	ATOM	659	CD1	ILE	389	20.431	9.383	25.683	1.00	25.45
	ATOM	660	C	ILE	389	21.694	5.401	27.349	1.00	26.54
	ATOM	661	O	ILE	389	20.938	5.631	28.294	1.00	22.58
65	ATOM	662	N	GLY	390	21.679	4.247	26.687	1.00	27.14
	ATOM	663	CA	GLY	390	20.753	3.201	27.090	1.00	28.42
	ATOM	664	C	GLY	390	21.133	2.719	28.482	1.00	29.67
	ATOM	665	O	GLY	390	20.275	2.521	29.348	1.00	29.21
70	ATOM	666	N	LEU	391	22.433	2.547	28.699	1.00	26.06
	ATOM	667	CA	LEU	391	22.955	2.091	29.983	1.00	29.23
	ATOM	668	CB	LEU	391	24.476	1.937	29.899	1.00	28.37
	ATOM	669	CG	LEU	391	25.206	1.656	31.210	1.00	30.81
	ATOM	670	CD1	LEU	391	24.717	0.332	31.793	1.00	25.73

						26.709	1.619	30.958	1.00	25.25
5	ATOM	671	CD2	LEU	391	22.603	3.070	31.104	1.00	30.84
	ATOM	672	C	LEU	391	22.156	2.669	32.186	1.00	29.19
	ATOM	673	O	LEU	391	22.817	4.355	30.850	1.00	28.91
	ATOM	674	N	VAL	392	22.506	5.369	31.851	1.00	28.86
	ATOM	675	CA	VAL	392	22.923	6.770	31.353	1.00	30.08
10	ATOM	676	CB	VAL	392	22.329	7.854	32.237	1.00	32.32
	ATOM	677	CG1	VAL	392	24.442	6.870	31.372	1.00	28.52
	ATOM	678	CG2	VAL	392	21.013	5.327	32.165	1.00	28.42
	ATOM	679	C	VAL	392	20.621	5.345	33.327	1.00	30.38
	ATOM	680	O	VAL	392	20.191	5.241	31.125	1.00	28.23
15	ATOM	681	N	TRP	393	18.732	5.186	31.280	1.00	29.70
	ATOM	682	CA	TRP	393	18.066	5.046	29.906	1.00	30.09
	ATOM	683	CB	TRP	393	16.605	4.670	29.953	1.00	33.50
	ATOM	684	CG	TRP	393	15.516	5.499	30.369	1.00	31.76
	ATOM	685	CD2	TRP	393	14.336	4.725	30.264	1.00	38.11
20	ATOM	686	CE2	TRP	393	15.419	6.821	30.824	1.00	32.56
	ATOM	687	CE3	TRP	393	16.057	3.459	29.618	1.00	34.31
	ATOM	688	CD1	TRP	393	14.696	3.486	29.801	1.00	34.36
	ATOM	689	NE1	TRP	393	13.073	5.233	30.597	1.00	37.93
	ATOM	690	CZ2	TRP	393	14.162	7.326	31.155	1.00	35.24
25	ATOM	691	CZ3	TRP	393	13.007	6.531	31.039	1.00	37.77
	ATOM	692	CH2	TRP	393	18.256	4.051	32.191	1.00	32.07
	ATOM	693	C	TRP	393	17.460	4.275	33.109	1.00	32.12
	ATOM	694	O	TRP	393	18.738	2.837	31.957	1.00	31.90
	ATOM	695	N	ARG	394	18.288	1.729	32.787	1.00	36.63
30	ATOM	696	CA	ARG	394	18.492	0.389	32.065	1.00	36.41
	ATOM	697	CB	ARG	394	19.914	0.009	31.764	1.00	36.50
	ATOM	698	CG	ARG	394	19.929	-1.132	30.748	1.00	36.34
	ATOM	699	CD	ARG	394	21.282	-1.561	30.417	1.00	33.97
	ATOM	700	NE	ARG	394	21.864	-1.350	29.239	1.00	31.61
35	ATOM	701	CZ	ARG	394	21.208	-0.715	28.281	1.00	32.42
	ATOM	702	NH1	ARG	394	23.098	-1.784	29.022	1.00	29.81
	ATOM	703	NH2	ARG	394	18.911	1.697	34.180	1.00	36.69
	ATOM	704	C	ARG	394	18.445	0.966	35.048	1.00	37.07
	ATOM	705	O	ARG	394	19.954	2.492	34.395	1.00	33.63
40	ATOM	706	N	SER	395	20.603	2.564	35.701	1.00	35.69
	ATOM	707	CA	SER	395	22.112	2.784	35.540	1.00	32.94
	ATOM	708	CB	SER	395	22.696	1.811	34.688	1.00	32.37
	ATOM	709	OG	SER	395	20.010	3.713	36.531	1.00	36.44
	ATOM	710	C	SER	395	20.389	3.916	37.687	1.00	38.68
45	ATOM	711	O	SER	395	19.076	4.449	35.937	1.00	36.46
	ATOM	712	N	MET	396	18.431	5.588	36.589	1.00	43.08
	ATOM	713	CA	MET	396	17.275	6.104	35.725	1.00	43.87
	ATOM	714	CB	MET	396	17.481	7.507	35.176	1.00	46.18
	ATOM	715	CG	MET	396	15.962	8.278	34.581	1.00	49.58
50	ATOM	716	SD	MET	396	14.988	8.298	36.065	1.00	53.58
	ATOM	717	CE	MET	396	17.906	5.303	37.992	1.00	46.18
	ATOM	718	C	MET	396	18.125	6.089	38.913	1.00	46.34
	ATOM	719	O	MET	396	17.215	4.180	38.152	1.00	49.39
	ATOM	720	N	GLU	397	16.645	3.821	39.444	1.00	52.12
55	ATOM	721	CA	GLU	397	15.296	3.130	39.246	1.00	55.34
	ATOM	722	CB	GLU	397	14.166	4.073	38.873	1.00	58.86
	ATOM	723	CG	GLU	397	13.195	3.448	37.891	1.00	63.28
	ATOM	724	CD	GLU	397	13.660	2.925	36.854	1.00	64.68
	ATOM	725	OE1	GLU	397	11.972	3.475	38.155	1.00	65.39
60	ATOM	726	OE2	GLU	397	17.548	2.933	40.283	1.00	52.75
	ATOM	727	C	GLU	397					

5	ATOM	728	O	GLU	397	17.071	2.187	41.139	1.00	53.96
	ATOM	729	N	HIS	398	18.851	3.014	40.040	1.00	50.25
	ATOM	730	CA	HIS	398	19.813	2.220	40.792	1.00	49.34
	ATOM	731	CB	HIS	398	20.271	1.018	39.963	1.00	52.04
	ATOM	732	CG	HIS	398	19.187	0.017	39.721	1.00	53.95
10	ATOM	733	CD2	HIS	398	18.750	-1.022	40.472	1.00	53.92
	ATOM	734	ND1	HIS	398	18.374	0.054	38.608	1.00	55.91
	ATOM	735	CE1	HIS	398	17.482	-0.917	38.685	1.00	55.53
	ATOM	736	NE2	HIS	398	17.688	-1.585	39.806	1.00	55.81
	ATOM	737	C	HIS	398	20.999	3.084	41.196	1.00	47.44
15	ATOM	738	O	HIS	398	22.121	2.887	40.730	1.00	44.91
	ATOM	739	N	PRO	399	20.755	4.049	42.096	1.00	46.45
	ATOM	740	CD	PRO	399	19.443	4.300	42.721	1.00	47.27
	ATOM	741	CA	PRO	399	21.785	4.968	42.586	1.00	45.35
	ATOM	742	CB	PRO	399	21.127	5.631	43.793	1.00	47.40
20	ATOM	743	CG	PRO	399	19.660	5.561	43.504	1.00	47.72
	ATOM	744	C	PRO	399	23.086	4.270	42.958	1.00	44.70
	ATOM	745	O	PRO	399	23.078	3.233	43.627	1.00	46.46
	ATOM	746	N	GLY	400	24.202	4.840	42.509	1.00	41.57
	ATOM	747	CA	GLY	400	25.506	4.281	42.813	1.00	39.84
25	ATOM	748	C	GLY	400	25.907	3.047	42.022	1.00	37.85
	ATOM	749	O	GLY	400	27.027	2.560	42.176	1.00	40.48
	ATOM	750	N	LYS	401	25.012	2.537	41.180	1.00	36.39
	ATOM	751	CA	LYS	401	25.315	1.344	40.390	1.00	34.47
	ATOM	752	CB	LYS	401	24.562	0.130	40.947	1.00	36.12
30	ATOM	753	CG	LYS	401	24.633	-0.007	42.466	1.00	39.30
	ATOM	754	CD	LYS	401	24.288	-1.429	42.903	1.00	44.38
	ATOM	755	CE	LYS	401	24.459	-1.605	44.408	1.00	46.68
	ATOM	756	NZ	LYS	401	24.968	-2.969	44.747	1.00	53.37
	ATOM	757	C	LYS	401	24.969	1.485	38.911	1.00	32.34
35	ATOM	758	O	LYS	401	24.141	2.308	38.531	1.00	31.16
	ATOM	759	N	LEU	402	25.612	0.663	38.086	1.00	28.52
	ATOM	760	CA	LEU	402	25.358	0.658	36.648	1.00	29.06
	ATOM	761	CB	LEU	402	26.661	0.847	35.867	1.00	29.26
	ATOM	762	CG	LEU	402	27.278	2.242	36.029	1.00	24.67
40	ATOM	763	CD1	LEU	402	28.623	2.310	35.310	1.00	27.47
	ATOM	764	CD2	LEU	402	26.312	3.277	35.482	1.00	24.93
	ATOM	765	C	LEU	402	24.755	-0.686	36.292	1.00	30.43
	ATOM	766	O	LEU	402	25.367	-1.727	36.535	1.00	31.36
	ATOM	767	N	LEU	403	23.552	-0.658	35.735	1.00	31.07
45	ATOM	768	CA	LEU	403	22.873	-1.880	35.335	1.00	32.96
	ATOM	769	CB	LEU	403	21.361	-1.693	35.434	1.00	33.86
	ATOM	770	CG	LEU	403	20.551	-2.991	35.415	1.00	39.29
	ATOM	771	CD1	LEU	403	20.584	-3.637	36.806	1.00	43.62
	ATOM	772	CD2	LEU	403	19.128	-2.689	34.998	1.00	41.32
50	ATOM	773	C	LEU	403	23.255	-2.218	33.899	1.00	30.06
	ATOM	774	O	LEU	403	22.543	-1.870	32.956	1.00	31.63
	ATOM	775	N	PHE	404	24.383	-2.893	33.733	1.00	29.19
	ATOM	776	CA	PHE	404	24.834	-3.256	32.403	1.00	28.93
	ATOM	777	CB	PHE	404	26.201	-3.929	32.493	1.00	30.05
55	ATOM	778	CG	PHE	404	27.305	-2.998	32.926	1.00	30.78
	ATOM	779	CD1	PHE	404	27.794	-3.033	34.228	1.00	32.91
	ATOM	780	CD2	PHE	404	27.848	-2.078	32.030	1.00	32.75
	ATOM	781	CE1	PHE	404	28.816	-2.160	34.638	1.00	34.73
	ATOM	782	CE2	PHE	404	28.864	-1.205	32.423	1.00	30.68
60	ATOM	783	CZ	PHE	404	29.350	-1.242	33.727	1.00	31.43
	ATOM	784	C	PHE	404	23.809	-4.181	31.756	1.00	30.80

5	ATOM	785	O	PHE	404	23.625	-4.175	30.538	1.00	28.09
	ATOM	786	N	ALA	405	23.138	-4.967	32.594	1.00	30.25
	ATOM	787	CA	ALA	405	22.104	-5.910	32.163	1.00	29.78
	ATOM	788	CB	ALA	405	22.745	-7.172	31.598	1.00	29.97
	ATOM	789	C	ALA	405	21.309	-6.237	33.429	1.00	31.95
10	ATOM	790	O	ALA	405	21.785	-5.995	34.535	1.00	32.36
	ATOM	791	N	PRO	406	20.088	-6.779	33.288	1.00	34.40
	ATOM	792	CD	PRO	406	19.356	-7.102	32.053	1.00	35.81
	ATOM	793	CA	PRO	406	19.303	-7.101	34.490	1.00	36.41
	ATOM	794	CB	PRO	406	17.985	-7.654	33.935	1.00	35.38
15	ATOM	795	CG	PRO	406	17.922	-7.153	32.519	1.00	36.49
	ATOM	796	C	PRO	406	19.997	-8.084	35.433	1.00	37.32
	ATOM	797	O	PRO	406	19.698	-8.112	36.626	1.00	38.34
	ATOM	798	N	ASN	407	20.924	-8.877	34.902	1.00	36.69
	ATOM	799	CA	ASN	407	21.652	-9.847	35.712	1.00	38.85
20	ATOM	800	CB	ASN	407	21.582	-11.243	35.083	1.00	39.69
	ATOM	801	CG	ASN	407	22.232	-11.306	33.711	1.00	44.10
	ATOM	802	OD1	ASN	407	22.345	-10.296	33.009	1.00	37.78
	ATOM	803	ND2	ASN	407	22.660	-12.503	33.319	1.00	45.74
	ATOM	804	C	ASN	407	23.100	-9.435	35.874	1.00	38.12
25	ATOM	805	O	ASN	407	23.965	-10.256	36.178	1.00	39.81
	ATOM	806	N	LEU	408	23.364	-8.149	35.671	1.00	37.80
	ATOM	807	CA	LEU	408	24.713	-7.631	35.799	1.00	36.89
	ATOM	808	CB	LEU	408	25.449	-7.720	34.459	1.00	36.09
	ATOM	809	CG	LEU	408	26.972	-7.609	34.550	1.00	35.08
30	ATOM	810	CD1	LEU	408	27.525	-8.775	35.354	1.00	39.15
	ATOM	811	CD2	LEU	408	27.578	-7.587	33.158	1.00	36.85
	ATOM	812	C	LEU	408	24.670	-6.187	36.286	1.00	40.55
	ATOM	813	O	LEU	408	24.646	-5.248	35.491	1.00	38.29
	ATOM	814	N	LEU	409	24.644	-6.034	37.607	1.00	39.50
35	ATOM	815	CA	LEU	409	24.606	-4.733	38.257	1.00	41.00
	ATOM	816	CB	LEU	409	23.392	-4.658	39.184	1.00	43.69
	ATOM	817	CG	LEU	409	23.164	-3.382	39.993	1.00	47.35
	ATOM	818	CD1	LEU	409	22.848	-2.233	39.058	1.00	47.09
	ATOM	819	CD2	LEU	409	22.014	-3.603	40.976	1.00	49.38
40	ATOM	820	C	LEU	409	25.894	-4.566	39.060	1.00	41.80
	ATOM	821	O	LEU	409	26.178	-5.358	39.960	1.00	41.00
	ATOM	822	N	LEU	410	26.676	-3.544	38.727	1.00	39.23
	ATOM	823	CA	LEU	410	27.931	-3.296	39.423	1.00	40.45
	ATOM	824	CB	LEU	410	29.106	-3.354	38.442	1.00	41.59
45	ATOM	825	CG	LEU	410	29.457	-4.660	37.716	1.00	44.87
	ATOM	826	CD1	LEU	410	30.972	-4.728	37.554	1.00	45.41
	ATOM	827	CD2	LEU	410	28.949	-5.872	38.484	1.00	47.02
	ATOM	828	C	LEU	410	27.946	-1.944	40.132	1.00	40.67
	ATOM	829	O	LEU	410	27.361	-0.970	39.652	1.00	40.22
50	ATOM	830	N	ASP	411	28.610	-1.890	41.281	1.00	41.57
	ATOM	831	CA	ASP	411	28.717	-0.640	42.025	1.00	42.69
	ATOM	832	CB	ASP	411	28.490	-0.874	43.528	1.00	44.44
	ATOM	833	CG	ASP	411	29.655	-1.578	44.210	1.00	46.70
	ATOM	834	OD1	ASP	411	29.537	-1.849	45.426	1.00	51.44
55	ATOM	835	OD2	ASP	411	30.680	-1.861	43.553	1.00	48.79
	ATOM	836	C	ASP	411	30.088	-0.016	41.779	1.00	43.70
	ATOM	837	O	ASP	411	30.933	-0.610	41.107	1.00	38.48
	ATOM	838	N	ARG	412	30.295	1.181	42.321	1.00	46.78
	ATOM	839	CA	ARG	412	31.554	1.905	42.171	1.00	49.97
60	ATOM	840	CB	ARG	412	31.601	3.090	43.138	1.00	51.28
	ATOM	841	CG	ARG	412	30.971	4.364	42.614	1.00	54.77



5	ATOM	842	CD	ARG	412	31.644	5.580	43.219	1.00	54.61
	ATOM	843	NE	ARG	412	33.071	5.615	42.912	1.00	56.53
	ATOM	844	CZ	ARG	412	33.827	6.708	42.985	1.00	61.90
	ATOM	845	NH1	ARG	412	33.291	7.866	43.356	1.00	63.48
	ATOM	846	NH2	ARG	412	35.120	6.645	42.682	1.00	61.21
10	ATOM	847	C	ARG	412	32.771	1.026	42.429	1.00	50.29
	ATOM	848	O	ARG	412	33.628	0.866	41.561	1.00	51.02
	ATOM	849	N	ASN	413	32.844	0.469	43.633	1.00	51.94
	ATOM	850	CA	ASN	413	33.969	-0.375	44.021	1.00	53.15
	ATOM	851	CB	ASN	413	33.719	-0.980	45.403	1.00	55.88
15	ATOM	852	CG	ASN	413	33.654	0.073	46.496	1.00	57.99
	ATOM	853	OD1	ASN	413	33.697	1.276	46.223	1.00	58.27
	ATOM	854	ND2	ASN	413	33.551	-0.375	47.742	1.00	57.90
	ATOM	855	C	ASN	413	34.235	-1.480	43.013	1.00	53.95
	ATOM	856	O	ASN	413	35.386	-1.743	42.659	1.00	53.67
20	ATOM	857	N	GLN	414	33.173	-2.129	42.547	1.00	55.33
	ATOM	858	CA	GLN	414	33.326	-3.198	41.573	1.00	55.42
	ATOM	859	CB	GLN	414	31.991	-3.904	41.343	1.00	55.44
	ATOM	860	CG	GLN	414	31.645	-4.933	42.391	1.00	56.07
	ATOM	861	CD	GLN	414	30.203	-5.376	42.336	1.00	57.40
25	ATOM	862	OE1	GLN	414	29.296	-4.536	42.402	1.00	60.22
	ATOM	863	NE2	GLN	414	29.973	-6.664	42.199	1.00	57.27
	ATOM	864	C	GLN	414	33.850	-2.630	40.259	1.00	55.51
	ATOM	865	O	GLN	414	34.654	-3.265	39.578	1.00	56.16
	ATOM	866	N	GLY	415	33.398	-1.430	39.910	1.00	57.07
30	ATOM	867	CA	GLY	415	33.849	-0.806	38.680	1.00	58.51
	ATOM	868	C	GLY	415	35.350	-0.582	38.689	1.00	61.10
	ATOM	869	O	GLY	415	36.023	-0.748	37.671	1.00	59.47
	ATOM	870	N	LYS	416	35.877	-0.211	39.851	1.00	62.77
	ATOM	871	CA	LYS	416	37.305	0.041	40.011	1.00	65.49
35	ATOM	872	CB	LYS	416	37.634	0.262	41.491	1.00	66.04
	ATOM	873	CG	LYS	416	38.121	1.663	41.823	1.00	68.71
	ATOM	874	CD	LYS	416	37.078	2.439	42.613	1.00	70.98
	ATOM	875	CE	LYS	416	37.404	2.448	44.100	1.00	71.84
	ATOM	876	NZ	LYS	416	36.225	2.079	44.933	1.00	71.95
40	ATOM	877	C	LYS	416	38.159	-1.105	39.472	1.00	66.41
	ATOM	878	O	LYS	416	39.361	-0.946	39.269	1.00	67.15
	ATOM	879	N	CYS	417	37.538	-2.257	39.238	1.00	67.33
	ATOM	880	CA	CYS	417	38.270	-3.414	38.741	1.00	68.16
	ATOM	881	CB	CYS	417	37.951	-4.642	39.602	1.00	70.88
45	ATOM	882	SG	CYS	417	38.592	-4.549	41.301	1.00	76.09
	ATOM	883	C	CYS	417	38.015	-3.736	37.270	1.00	67.54
	ATOM	884	O	CYS	417	38.632	-4.653	36.720	1.00	68.48
	ATOM	885	N	VAL	418	37.111	-2.994	36.631	1.00	64.67
	ATOM	886	CA	VAL	418	36.817	-3.226	35.218	1.00	59.97
50	ATOM	887	CB	VAL	418	35.326	-2.917	34.879	1.00	59.60
	ATOM	888	CG1	VAL	418	34.971	-1.503	35.284	1.00	59.13
	ATOM	889	CG2	VAL	418	35.072	-3.121	33.391	1.00	54.85
	ATOM	890	C	VAL	418	37.739	-2.362	34.355	1.00	58.37
	ATOM	891	O	VAL	418	37.799	-1.140	34.512	1.00	55.44
55	ATOM	892	N	GLU	419	38.463	-3.012	33.450	1.00	56.02
	ATOM	893	CA	GLU	419	39.403	-2.328	32.570	1.00	54.28
	ATOM	894	CB	GLU	419	40.149	-3.351	31.710	1.00	57.57
	ATOM	895	CG	GLU	419	39.385	-3.779	30.468	1.00	60.87
	ATOM	896	CD	GLU	419	40.179	-4.722	29.584	1.00	63.34
60	ATOM	897	OE1	GLU	419	40.432	-5.870	30.011	1.00	64.90
	ATOM	898	OE2	GLU	419	40.546	-4.313	28.462	1.00	63.18

5	ATOM	899	C	GLU	419	38.761	-1.281	31.662	1.00	52.05
	ATOM	900	O	GLU	419	37.665	-1.481	31.131	1.00	49.82
	ATOM	901	N	GLY	420	39.465	-0.165	31.491	1.00	49.45
	ATOM	902	CA	GLY	420	38.983	0.908	30.642	1.00	46.22
	ATOM	903	C	GLY	420	37.895	1.767	31.254	1.00	44.55
10	ATOM	904	O	GLY	420	37.417	2.705	30.619	1.00	42.08
	ATOM	905	N	MET	421	37.503	1.471	32.488	1.00	43.41
	ATOM	906	CA	MET	421	36.449	2.248	33.123	1.00	42.48
	ATOM	907	CB	MET	421	35.306	1.327	33.554	1.00	42.34
	ATOM	908	CG	MET	421	34.590	0.635	32.396	1.00	38.22
15	ATOM	909	SD	MET	421	32.927	0.102	32.843	1.00	38.56
	ATOM	910	CE	MET	421	32.003	1.699	32.766	1.00	35.54
	ATOM	911	C	MET	421	36.923	3.059	34.312	1.00	41.64
	ATOM	912	O	MET	421	36.113	3.512	35.111	1.00	39.77
	ATOM	913	N	VAL	422	38.232	3.256	34.430	1.00	43.42
20	ATOM	914	CA	VAL	422	38.757	4.019	35.557	1.00	44.79
	ATOM	915	CB	VAL	422	40.285	4.248	35.433	1.00	46.54
	ATOM	916	CG1	VAL	422	40.595	5.086	34.206	1.00	48.25
	ATOM	917	CG2	VAL	422	40.813	4.920	36.696	1.00	46.24
	ATOM	918	C	VAL	422	38.056	5.372	35.689	1.00	44.09
25	ATOM	919	O	VAL	422	37.691	5.783	36.783	1.00	44.12
	ATOM	920	N	GLU	423	37.846	6.055	34.570	1.00	42.07
	ATOM	921	CA	GLU	423	37.192	7.356	34.616	1.00	40.24
	ATOM	922	CB	GLU	423	37.909	8.338	33.684	1.00	44.02
	ATOM	923	CG	GLU	423	39.411	8.467	33.893	1.00	50.04
30	ATOM	924	CD	GLU	423	40.096	9.158	32.719	1.00	55.64
	ATOM	925	OE1	GLU	423	39.539	10.156	32.205	1.00	56.66
	ATOM	926	OE2	GLU	423	41.188	8.703	32.306	1.00	58.02
	ATOM	927	C	GLU	423	35.704	7.337	34.250	1.00	35.77
	ATOM	928	O	GLU	423	34.881	7.955	34.919	1.00	33.20
35	ATOM	929	N	ILE	424	35.345	6.617	33.197	1.00	36.16
	ATOM	930	CA	ILE	424	33.949	6.643	32.771	1.00	31.63
	ATOM	931	CB	ILE	424	33.803	6.087	31.347	1.00	33.58
	ATOM	932	CG2	ILE	424	34.639	6.936	30.395	1.00	33.48
	ATOM	933	CG1	ILE	424	34.204	4.617	31.296	1.00	34.46
40	ATOM	934	CD1	ILE	424	33.857	3.955	29.978	1.00	34.67
	ATOM	935	C	ILE	424	32.890	6.035	33.685	1.00	28.89
	ATOM	936	O	ILE	424	31.729	6.443	33.632	1.00	26.49
	ATOM	937	N	PHE	425	33.261	5.091	34.542	1.00	29.26
	ATOM	938	CA	PHE	425	32.257	4.520	35.447	1.00	29.87
45	ATOM	939	CB	PHE	425	32.903	3.529	36.423	1.00	31.26
	ATOM	940	CG	PHE	425	31.948	2.496	36.959	1.00	32.17
	ATOM	941	CD1	PHE	425	31.124	2.783	38.048	1.00	33.70
	ATOM	942	CD2	PHE	425	31.881	1.230	36.381	1.00	30.64
	ATOM	943	CE1	PHE	425	30.244	1.814	38.563	1.00	32.60
50	ATOM	944	CE2	PHE	425	31.010	0.256	36.881	1.00	31.55
	ATOM	945	CZ	PHE	425	30.189	0.549	37.973	1.00	33.34
	ATOM	946	C	PHE	425	31.594	5.649	36.240	1.00	30.17
	ATOM	947	O	PHE	425	30.368	5.774	36.276	1.00	26.71
	ATOM	948	N	ASP	426	32.415	6.483	36.870	1.00	29.45
55	ATOM	949	CA	ASP	426	31.893	7.587	37.661	1.00	32.29
	ATOM	950	CB	ASP	426	33.031	8.291	38.401	1.00	33.49
	ATOM	951	CG	ASP	426	33.455	7.546	39.655	1.00	39.42
	ATOM	952	OD1	ASP	426	32.767	6.574	40.038	1.00	38.35
	ATOM	953	OD2	ASP	426	34.480	7.934	40.256	1.00	39.58
60	ATOM	954	C	ASP	426	31.133	8.592	36.806	1.00	29.02
	ATOM	955	O	ASP	426	30.154	9.175	37.257	1.00	31.34

5	ATOM	956	N	MET	427	31.585	8.797	35.572	1.00	30.69
	ATOM	957	CA	MET	427	30.919	9.736	34.675	1.00	28.63
	ATOM	958	CB	MET	427	31.744	9.912	33.407	1.00	26.83
	ATOM	959	CG	MET	427	33.032	10.680	33.608	1.00	31.41
	ATOM	960	SD	MET	427	33.962	10.783	32.077	1.00	34.87
10	ATOM	961	CE	MET	427	35.409	11.753	32.643	1.00	44.60
	ATOM	962	C	MET	427	29.526	9.202	34.324	1.00	28.70
	ATOM	963	O	MET	427	28.536	9.947	34.302	1.00	25.01
	ATOM	964	N	LEU	428	29.451	7.902	34.057	1.00	25.13
	ATOM	965	CA	LEU	428	28.173	7.292	33.730	1.00	27.60
15	ATOM	966	CB	LEU	428	28.379	5.824	33.332	1.00	28.00
	ATOM	967	CG	LEU	428	29.039	5.682	31.957	1.00	26.99
	ATOM	968	CD1	LEU	428	29.678	4.303	31.782	1.00	27.80
	ATOM	969	CD2	LEU	428	27.995	5.927	30.894	1.00	25.33
	ATOM	970	C	LEU	428	27.210	7.412	34.916	1.00	29.59
20	ATOM	971	O	LEU	428	26.041	7.743	34.743	1.00	27.07
	ATOM	972	N	LEU	429	27.701	7.147	36.126	1.00	30.40
	ATOM	973	CA	LEU	429	26.859	7.251	37.323	1.00	30.59
	ATOM	974	CB	LEU	429	27.675	6.884	38.571	1.00	31.76
	ATOM	975	CG	LEU	429	28.078	5.415	38.757	1.00	32.43
25	ATOM	976	CD1	LEU	429	28.961	5.264	39.995	1.00	31.60
	ATOM	977	CD2	LEU	429	26.825	4.573	38.903	1.00	34.66
	ATOM	978	C	LEU	429	26.319	8.681	37.466	1.00	30.46
	ATOM	979	O	LEU	429	25.143	8.901	37.769	1.00	28.40
	ATOM	980	N	ALA	430	27.193	9.656	37.237	1.00	31.34
30	ATOM	981	CA	ALA	430	26.806	11.059	37.332	1.00	29.83
	ATOM	982	CB	ALA	430	28.017	11.951	37.078	1.00	31.29
	ATOM	983	C	ALA	430	25.696	11.387	36.344	1.00	31.04
	ATOM	984	O	ALA	430	24.753	12.107	36.674	1.00	30.79
	ATOM	985	N	THR	431	25.802	10.854	35.128	1.00	30.30
35	ATOM	986	CA	THR	431	24.786	11.105	34.112	1.00	28.81
	ATOM	987	CB	THR	431	25.207	10.533	32.737	1.00	30.55
	ATOM	988	OG1	THR	431	26.569	10.893	32.465	1.00	31.88
	ATOM	989	CG2	THR	431	24.321	11.087	31.634	1.00	25.63
	ATOM	990	C	THR	431	23.462	10.481	34.530	1.00	29.49
40	ATOM	991	O	THR	431	22.402	11.099	34.397	1.00	26.18
	ATOM	992	N	SER	432	23.520	9.253	35.037	1.00	28.11
	ATOM	993	CA	SER	432	22.308	8.573	35.480	1.00	29.78
	ATOM	994	CB	SER	432	22.639	7.177	36.008	1.00	33.11
	ATOM	995	OG	SER	432	21.454	6.412	36.136	1.00	36.92
45	ATOM	996	C	SER	432	21.651	9.399	36.589	1.00	31.49
	ATOM	997	O	SER	432	20.433	9.576	36.613	1.00	30.09
	ATOM	998	N	ASER	433	22.476	9.901	37.496	0.75	32.09
	ATOM	999	N	BSER	433	22.474	9.906	37.500	0.25	31.10
	ATOM	1000	CA	ASER	433	22.002	10.715	38.605	0.75	35.68
50	ATOM	1001	CA	BSER	433	21.985	10.717	38.608	0.25	32.21
	ATOM	1002	CB	ASER	433	23.185	11.097	39.502	0.75	37.18
	ATOM	1003	CB	BSER	433	23.145	11.104	39.529	0.25	31.45
	ATOM	1004	OG	ASER	433	22.823	12.090	40.443	0.75	44.09
	ATOM	1005	OG	BSER	433	23.785	9.953	40.053	0.25	29.52
55	ATOM	1006	C	ASER	433	21.299	11.971	38.091	0.75	35.01
	ATOM	1007	C	BSER	433	21.295	11.976	38.092	0.25	32.88
	ATOM	1008	O	ASER	433	20.257	12.373	38.612	0.75	35.34
	ATOM	1009	O	BSER	433	20.264	12.391	38.622	0.25	33.42
	ATOM	1010	N	ARG	434	21.867	12.579	37.054	1.00	33.38
60	ATOM	1011	CA	ARG	434	21.300	13.788	36.470	1.00	34.19
	ATOM	1012	CB	ARG	434	22.239	14.354	35.400	1.00	33.89

5	ATOM	1013	CG	ARG	434	21.670	15.528	34.625	1.00	38.30
	ATOM	1014	CD	ARG	434	21.559	16.787	35.479	1.00	37.91
	ATOM	1015	NE	ARG	434	21.158	17.944	34.680	1.00	37.78
	ATOM	1016	CZ	ARG	434	20.488	18.995	35.149	1.00	41.06
	ATOM	1017	NH1	ARG	434	20.132	19.049	36.428	1.00	40.70
10	ATOM	1018	NH2	ARG	434	20.175	19.998	34.337	1.00	38.78
	ATOM	1019	C	ARG	434	19.937	13.491	35.873	1.00	33.48
	ATOM	1020	O	ARG	434	18.996	14.266	36.053	1.00	30.54
	ATOM	1021	N	PHE	435	19.831	12.371	35.158	1.00	34.68
	ATOM	1022	CA	PHE	435	18.563	11.963	34.549	1.00	35.02
15	ATOM	1023	CB	PHE	435	18.727	10.634	33.796	1.00	34.96
	ATOM	1024	CG	PHE	435	19.240	10.779	32.386	1.00	37.63
	ATOM	1025	CD1	PHE	435	19.459	12.035	31.824	1.00	42.03
	ATOM	1026	CD2	PHE	435	19.521	9.649	31.623	1.00	41.24
	ATOM	1027	CE1	PHE	435	19.953	12.164	30.521	1.00	43.11
20	ATOM	1028	CE2	PHE	435	20.016	9.768	30.322	1.00	40.59
	ATOM	1029	CZ	PHE	435	20.233	11.029	29.775	1.00	40.63
	ATOM	1030	C	PHE	435	17.527	11.780	35.657	1.00	35.49
	ATOM	1031	O	PHE	435	16.361	12.135	35.496	1.00	34.78
	ATOM	1032	N	ARG	436	17.968	11.216	36.777	1.00	38.27
25	ATOM	1033	CA	ARG	436	17.094	10.982	37.924	1.00	40.67
	ATOM	1034	CB	ARG	436	17.844	10.215	39.012	1.00	40.70
	ATOM	1035	CG	ARG	436	16.942	9.590	40.068	1.00	44.98
	ATOM	1036	CD	ARG	436	17.648	8.459	40.810	1.00	48.09
	ATOM	1037	NE	ARG	436	18.982	8.841	41.275	1.00	50.16
30	ATOM	1038	CZ	ARG	436	20.119	8.361	40.777	1.00	52.19
	ATOM	1039	NH1	ARG	436	20.099	7.472	39.790	1.00	49.34
	ATOM	1040	NH2	ARG	436	21.283	8.770	41.266	1.00	51.85
	ATOM	1041	C	ARG	436	16.576	12.302	38.493	1.00	40.40
	ATOM	1042	O	ARG	436	15.382	12.458	38.730	1.00	41.49
35	ATOM	1043	N	MET	437	17.477	13.252	38.706	1.00	40.02
	ATOM	1044	CA	MET	437	17.090	14.546	39.245	1.00	41.02
	ATOM	1045	CB	MET	437	18.329	15.427	39.440	1.00	40.29
	ATOM	1046	C	MET	437	16.099	15.221	38.299	1.00	40.81
	ATOM	1047	O	MET	437	15.111	15.805	38.734	1.00	42.46
40	ATOM	1048	N	MET	438	16.367	15.127	37.001	1.00	39.02
	ATOM	1049	CA	MET	438	15.510	15.732	35.988	1.00	40.11
	ATOM	1050	CB	MET	438	16.237	15.793	34.651	1.00	38.16
	ATOM	1051	CG	MET	438	17.352	16.794	34.601	1.00	41.52
	ATOM	1052	SD	MET	438	17.999	16.862	32.943	1.00	43.94
45	ATOM	1053	CE	MET	438	16.698	17.748	32.096	1.00	39.96
	ATOM	1054	C	MET	438	14.221	14.964	35.783	1.00	37.72
	ATOM	1055	O	MET	438	13.305	15.451	35.125	1.00	36.82
	ATOM	1056	N	ASN	439	14.155	13.759	36.337	1.00	38.81
	ATOM	1057	CA	ASN	439	12.981	12.919	36.174	1.00	40.77
50	ATOM	1058	CB	ASN	439	11.762	13.556	36.847	1.00	44.52
	ATOM	1059	CG	ASN	439	10.566	12.620	36.887	1.00	48.29
	ATOM	1060	OD1	ASN	439	10.721	11.400	36.964	1.00	48.48
	ATOM	1061	ND2	ASN	439	9.365	13.189	36.829	1.00	50.23
	ATOM	1062	C	ASN	439	12.725	12.744	34.677	1.00	39.36
55	ATOM	1063	O	ASN	439	11.637	13.037	34.172	1.00	37.76
	ATOM	1064	N	LEU	440	13.749	12.274	33.972	1.00	37.65
	ATOM	1065	CA	LEU	440	13.655	12.052	32.532	1.00	35.22
	ATOM	1066	CB	LEU	440	14.999	11.576	31.987	1.00	34.70
	ATOM	1067	CG	LEU	440	15.022	11.467	30.462	1.00	35.45
60	ATOM	1068	CD1	LEU	440	14.890	12.862	29.869	1.00	35.24
	ATOM	1069	CD2	LEU	440	16.297	10.795	29.999	1.00	35.30

5	ATOM	1070	C	LEU	440	12.587	11.024	32.196	1.00	36.48
	ATOM	1071	O	LEU	440	12.518	9.967	32.826	1.00	37.36
	ATOM	1072	N	GLN	441	11.763	11.328	31.197	1.00	36.82
	ATOM	1073	CA	GLN	441	10.696	10.420	30.785	1.00	38.51
	ATOM	1074	CB	GLN	441	9.431	11.211	30.443	1.00	38.23
10	ATOM	1075	CG	GLN	441	8.912	12.063	31.592	1.00	42.46
	ATOM	1076	CD	GLN	441	8.362	11.227	32.729	1.00	44.91
	ATOM	1077	OE1	GLN	441	7.268	10.668	32.629	1.00	47.31
	ATOM	1078	NE2	GLN	441	9.119	11.132	33.818	1.00	44.06
	ATOM	1079	C	GLN	441	11.099	9.565	29.585	1.00	38.48
15	ATOM	1080	O	GLN	441	11.923	9.976	28.763	1.00	35.80
	ATOM	1081	N	GLY	442	10.500	8.378	29.494	1.00	36.03
	ATOM	1082	CA	GLY	442	10.792	7.468	28.401	1.00	37.72
	ATOM	1083	C	GLY	442	10.599	8.112	27.043	1.00	36.88
	ATOM	1084	O	GLY	442	11.381	7.877	26.123	1.00	33.72
20	ATOM	1085	N	GLU	443	9.556	8.925	26.918	1.00	36.59
	ATOM	1086	CA	GLU	443	9.269	9.603	25.661	1.00	37.13
	ATOM	1087	CB	GLU	443	7.956	10.379	25.764	1.00	41.57
	ATOM	1088	CG	GLU	443	6.723	9.488	25.879	1.00	47.76
	ATOM	1089	CD	GLU	443	6.483	9.008	27.302	1.00	53.96
25	ATOM	1090	OE1	GLU	443	5.619	8.123	27.498	1.00	57.66
	ATOM	1091	OE2	GLU	443	7.159	9.515	28.225	1.00	56.13
	ATOM	1092	C	GLU	443	10.408	10.551	25.311	1.00	35.27
	ATOM	1093	O	GLU	443	10.759	10.704	24.145	1.00	33.85
	ATOM	1094	N	GLU	444	10.984	11.179	26.331	1.00	32.09
30	ATOM	1095	CA	GLU	444	12.097	12.095	26.126	1.00	33.92
	ATOM	1096	CB	GLU	444	12.332	12.924	27.388	1.00	34.97
	ATOM	1097	CG	GLU	444	11.169	13.845	27.732	1.00	38.28
	ATOM	1098	CD	GLU	444	11.383	14.610	29.023	1.00	38.11
	ATOM	1099	OE1	GLU	444	11.800	13.993	30.026	1.00	39.53
35	ATOM	1100	OE2	GLU	444	11.132	15.834	29.036	1.00	40.77
	ATOM	1101	C	GLU	444	13.356	11.305	25.770	1.00	33.59
	ATOM	1102	O	GLU	444	14.085	11.670	24.842	1.00	33.35
	ATOM	1103	N	PHE	445	13.590	10.215	26.501	1.00	30.68
	ATOM	1104	CA	PHE	445	14.753	9.357	26.276	1.00	32.49
40	ATOM	1105	CB	PHE	445	14.703	8.139	27.203	1.00	29.35
	ATOM	1106	CG	PHE	445	15.667	7.047	26.828	1.00	30.78
	ATOM	1107	CD1	PHE	445	17.036	7.201	27.030	1.00	28.25
	ATOM	1108	CD2	PHE	445	15.205	5.863	26.266	1.00	30.62
	ATOM	1109	CE1	PHE	445	17.933	6.195	26.675	1.00	28.67
45	ATOM	1110	CE2	PHE	445	16.095	4.848	25.908	1.00	31.37
	ATOM	1111	CZ	PHE	445	17.460	5.015	26.113	1.00	30.37
	ATOM	1112	C	PHE	445	14.850	8.885	24.829	1.00	31.11
	ATOM	1113	O	PHE	445	15.924	8.947	24.221	1.00	32.20
	ATOM	1114	N	VAL	446	13.739	8.415	24.266	1.00	28.63
50	ATOM	1115	CA	VAL	446	13.787	7.943	22.889	1.00	27.94
	ATOM	1116	CB	VAL	446	12.478	7.193	22.478	1.00	28.48
	ATOM	1117	CG1	VAL	446	12.318	5.939	23.343	1.00	29.61
	ATOM	1118	CG2	VAL	446	11.265	8.092	22.607	1.00	27.23
	ATOM	1119	C	VAL	446	14.099	9.064	21.900	1.00	27.28
55	ATOM	1120	O	VAL	446	14.781	8.837	20.904	1.00	28.07
	ATOM	1121	N	CYS	447	13.619	10.275	22.166	1.00	28.97
	ATOM	1122	CA	CYS	447	13.919	11.394	21.272	1.00	29.14
	ATOM	1123	CB	CYS	447	13.156	12.653	21.693	1.00	28.90
	ATOM	1124	SG	CYS	447	11.389	12.591	21.309	1.00	35.68
60	ATOM	1125	C	CYS	447	15.420	11.677	21.328	1.00	28.03
	ATOM	1126	O	CYS	447	16.063	11.885	20.302	1.00	29.34

5	ATOM	1127	N	LEU	448	15.969	11.686	22.538	1.00	27.28
	ATOM	1128	CA	LEU	448	17.392	11.938	22.729	1.00	25.30
	ATOM	1129	CB	LEU	448	17.733	11.932	24.220	1.00	27.72
	ATOM	1130	CG	LEU	448	17.248	13.135	25.040	1.00	29.54
	ATOM	1131	CD1	LEU	448	17.807	13.042	26.454	1.00	30.85
10	ATOM	1132	CD2	LEU	448	17.688	14.434	24.376	1.00	30.24
	ATOM	1133	C	LEU	448	18.245	10.902	22.008	1.00	27.62
	ATOM	1134	O	LEU	448	19.207	11.252	21.327	1.00	25.10
	ATOM	1135	N	LYS	449	17.905	9.621	22.162	1.00	25.16
	ATOM	1136	CA	LYS	449	18.673	8.570	21.506	1.00	27.55
15	ATOM	1137	CB	LYS	449	18.135	7.185	21.900	1.00	28.99
	ATOM	1138	CG	LYS	449	19.134	6.052	21.694	1.00	34.70
	ATOM	1139	CD	LYS	449	18.737	4.789	22.459	1.00	32.67
	ATOM	1140	CE	LYS	449	17.267	4.419	22.220	1.00	31.87
	ATOM	1141	NZ	LYS	449	17.022	2.967	22.472	1.00	29.14
20	ATOM	1142	C	LYS	449	18.626	8.749	19.990	1.00	25.88
	ATOM	1143	O	LYS	449	19.610	8.489	19.296	1.00	25.93
	ATOM	1144	N	SER	450	17.482	9.197	19.480	1.00	26.07
	ATOM	1145	CA	SER	450	17.323	9.421	18.052	1.00	27.24
	ATOM	1146	CB	SER	450	15.857	9.705	17.721	1.00	32.24
25	ATOM	1147	OG	SER	450	15.098	8.519	17.779	1.00	34.94
	ATOM	1148	C	SER	450	18.176	10.607	17.618	1.00	26.78
	ATOM	1149	O	SER	450	18.763	10.598	16.535	1.00	25.85
	ATOM	1150	N	ILE	451	18.231	11.632	18.463	1.00	26.94
	ATOM	1151	CA	ILE	451	19.032	12.810	18.155	1.00	26.13
30	ATOM	1152	CB	ILE	451	18.950	13.850	19.291	1.00	27.72
	ATOM	1153	CG2	ILE	451	20.019	14.929	19.101	1.00	20.53
	ATOM	1154	CG1	ILE	451	17.553	14.475	19.322	1.00	29.49
	ATOM	1155	CD1	ILE	451	17.377	15.473	20.447	1.00	36.24
	ATOM	1156	C	ILE	451	20.489	12.381	17.989	1.00	24.88
35	ATOM	1157	O	ILE	451	21.161	12.771	17.034	1.00	26.96
	ATOM	1158	N	ILE	452	20.977	11.582	18.931	1.00	22.72
	ATOM	1159	CA	ILE	452	22.359	11.120	18.880	1.00	21.95
	ATOM	1160	CB	ILE	452	22.660	10.155	20.050	1.00	23.57
	ATOM	1161	CG2	ILE	452	23.982	9.435	19.804	1.00	22.10
40	ATOM	1162	CG1	ILE	452	22.718	10.949	21.371	1.00	21.70
	ATOM	1163	CD1	ILE	452	22.768	10.060	22.624	1.00	25.30
	ATOM	1164	C	ILE	452	22.656	10.419	17.557	1.00	23.02
	ATOM	1165	O	ILE	452	23.650	10.708	16.885	1.00	21.25
	ATOM	1166	N	LEU	453	21.779	9.497	17.173	1.00	22.83
45	ATOM	1167	CA	LEU	453	21.984	8.768	15.935	1.00	22.05
	ATOM	1168	CB	LEU	453	20.843	7.764	15.733	1.00	22.06
	ATOM	1169	CG	LEU	453	20.712	7.189	14.324	1.00	22.03
	ATOM	1170	CD1	LEU	453	21.815	6.165	14.107	1.00	24.81
	ATOM	1171	CD2	LEU	453	19.328	6.535	14.156	1.00	24.73
50	ATOM	1172	C	LEU	453	22.092	9.687	14.717	1.00	23.95
	ATOM	1173	O	LEU	453	22.962	9.501	13.860	1.00	24.60
	ATOM	1174	N	LEU	454	21.220	10.687	14.638	1.00	26.72
	ATOM	1175	CA	LEU	454	21.234	11.599	13.494	1.00	26.45
	ATOM	1176	CB	LEU	454	19.852	12.242	13.330	1.00	25.51
55	ATOM	1177	CG	LEU	454	18.737	11.222	13.052	1.00	30.16
	ATOM	1178	CD1	LEU	454	17.405	11.926	12.955	1.00	28.76
	ATOM	1179	CD2	LEU	454	19.037	10.478	11.759	1.00	32.59
	ATOM	1180	C	LEU	454	22.292	12.703	13.552	1.00	28.24
	ATOM	1181	O	LEU	454	22.778	13.148	12.513	1.00	29.06
60	ATOM	1182	N	ASN	455	22.638	13.146	14.757	1.00	26.56
	ATOM	1183	CA	ASN	455	23.604	14.236	14.934	1.00	26.79

5	ATOM	1184	CB	ASN	455	23.284	14.998	16.224	1.00	26.20
	ATOM	1185	CG	ASN	455	24.174	16.217	16.419	1.00	27.26
	ATOM	1186	OD1	ASN	455	24.171	17.134	15.602	1.00	30.83
	ATOM	1187	ND2	ASN	455	24.931	16.230	17.506	1.00	27.16
	ATOM	1188	C	ASN	455	25.062	13.782	14.954	1.00	30.63
10	ATOM	1189	O	ASN	455	25.965	14.517	14.525	1.00	27.69
	ATOM	1190	N	SER	456	25.268	12.569	15.461	1.00	30.48
	ATOM	1191	CA	SER	456	26.572	11.928	15.579	1.00	35.26
	ATOM	1192	CB	SER	456	26.393	10.393	15.505	1.00	39.69
	ATOM	1193	OG	SER	456	25.871	9.953	14.243	1.00	30.73
15	ATOM	1194	C	SER	456	27.627	12.344	14.562	1.00	35.56
	ATOM	1195	O	SER	456	28.599	13.041	14.884	1.00	33.00
	ATOM	1196	N	GLY	457	27.437	11.886	13.334	1.00	33.88
	ATOM	1197	CA	GLY	457	28.393	12.189	12.292	1.00	36.77
	ATOM	1198	C	GLY	457	27.876	13.017	11.136	1.00	37.02
20	ATOM	1199	O	GLY	457	28.310	12.805	10.013	1.00	38.66
	ATOM	1200	N	VAL	458	26.967	13.956	11.392	1.00	39.12
	ATOM	1201	CA	VAL	458	26.438	14.802	10.317	1.00	43.81
	ATOM	1202	CB	VAL	458	25.231	15.648	10.755	1.00	44.25
	ATOM	1203	CG1	VAL	458	24.209	15.713	9.631	1.00	44.51
25	ATOM	1204	CG2	VAL	458	24.638	15.098	12.013	1.00	50.53
	ATOM	1205	C	VAL	458	27.472	15.801	9.817	1.00	46.72
	ATOM	1206	O	VAL	458	27.391	16.265	8.681	1.00	47.08
	ATOM	1207	N	TYR	459	28.432	16.144	10.670	1.00	50.74
	ATOM	1208	CA	TYR	459	29.456	17.114	10.301	1.00	55.43
30	ATOM	1209	CB	TYR	459	29.647	18.129	11.433	1.00	56.62
	ATOM	1210	CG	TYR	459	28.375	18.870	11.781	1.00	59.34
	ATOM	1211	CD1	TYR	459	28.094	19.229	13.095	1.00	60.73
	ATOM	1212	CE1	TYR	459	26.900	19.867	13.429	1.00	62.14
	ATOM	1213	CD2	TYR	459	27.430	19.175	10.795	1.00	62.16
35	ATOM	1214	CE2	TYR	459	26.234	19.812	11.118	1.00	63.83
	ATOM	1215	CZ	TYR	459	25.976	20.154	12.437	1.00	62.88
	ATOM	1216	OH	TYR	459	24.790	20.764	12.767	1.00	62.56
	ATOM	1217	C	TYR	459	30.791	16.489	9.928	1.00	57.21
	ATOM	1218	O	TYR	459	31.793	17.189	9.798	1.00	56.86
40	ATOM	1219	N	THR	460	30.800	15.173	9.750	1.00	59.22
	ATOM	1220	CA	THR	460	32.018	14.474	9.366	1.00	62.25
	ATOM	1221	CB	THR	460	32.502	13.531	10.499	1.00	63.07
	ATOM	1222	OG1	THR	460	33.474	12.613	9.983	1.00	67.80
	ATOM	1223	CG2	THR	460	31.344	12.759	11.084	1.00	60.23
45	ATOM	1224	C	THR	460	31.759	13.678	8.086	1.00	63.54
	ATOM	1225	O	THR	460	32.457	12.708	7.782	1.00	63.91
	ATOM	1226	N	PHE	461	30.758	14.113	7.326	1.00	65.06
	ATOM	1227	CA	PHE	461	30.395	13.446	6.080	1.00	67.00
	ATOM	1228	CB	PHE	461	29.052	13.975	5.563	1.00	66.48
50	ATOM	1229	CG	PHE	461	27.867	13.147	5.991	1.00	66.30
	ATOM	1230	CD1	PHE	461	26.657	13.754	6.312	1.00	65.58
	ATOM	1231	CD2	PHE	461	27.963	11.760	6.085	1.00	66.41
	ATOM	1232	CE1	PHE	461	25.562	12.996	6.723	1.00	65.45
	ATOM	1233	CE2	PHE	461	26.872	10.994	6.494	1.00	66.83
55	ATOM	1234	CZ	PHE	461	25.670	11.616	6.814	1.00	65.12
	ATOM	1235	C	PHE	461	31.463	13.604	5.004	1.00	68.38
	ATOM	1236	O	PHE	461	32.181	14.606	4.962	1.00	68.98
	ATOM	1237	N	LEU	462	31.542	12.601	4.132	1.00	69.57
	ATOM	1238	CA	LEU	462	32.511	12.545	3.039	1.00	71.68
60	ATOM	1239	CB	LEU	462	32.080	11.475	2.030	1.00	71.00
	ATOM	1240	C	LEU	462	32.810	13.856	2.304	1.00	72.40

5	ATOM	1241	O	LEU	462	33.725	14.590	2.680	1.00	73.45
	ATOM	1242	N	SER	463	32.043	14.141	1.253	1.00	73.22
	ATOM	1243	CA	SER	463	32.262	15.343	0.449	1.00	72.61
	ATOM	1244	CB	SER	463	32.544	14.942	-1.005	1.00	73.38
	ATOM	1245	C	SER	463	31.126	16.362	0.491	1.00	71.17
10	ATOM	1246	O	SER	463	30.455	16.528	1.511	1.00	72.05
	ATOM	1247	N	SER	464	30.932	17.049	-0.633	1.00	68.86
	ATOM	1248	CA	SER	464	29.892	18.063	-0.759	1.00	66.06
	ATOM	1249	CB	SER	464	30.514	19.457	-0.704	1.00	66.26
	ATOM	1250	C	SER	464	29.108	17.887	-2.060	1.00	63.72
15	ATOM	1251	O	SER	464	28.657	18.862	-2.662	1.00	62.88
	ATOM	1252	N	THR	465	28.954	16.638	-2.493	1.00	60.93
	ATOM	1253	CA	THR	465	28.205	16.343	-3.709	1.00	57.47
	ATOM	1254	CB	THR	465	28.185	14.824	-4.004	1.00	57.80
	ATOM	1255	OG1	THR	465	27.525	14.135	-2.934	1.00	54.75
20	ATOM	1256	CG2	THR	465	29.606	14.287	-4.149	1.00	57.49
	ATOM	1257	C	THR	465	26.767	16.824	-3.523	1.00	54.93
	ATOM	1258	O	THR	465	26.349	17.129	-2.407	1.00	54.26
	ATOM	1259	N	LEU	466	26.013	16.892	-4.614	1.00	51.85
	ATOM	1260	CA	LEU	466	24.625	17.330	-4.550	1.00	49.25
25	ATOM	1261	CB	LEU	466	24.013	17.349	-5.956	1.00	48.74
	ATOM	1262	CG	LEU	466	22.953	18.415	-6.253	1.00	48.72
	ATOM	1263	CD1	LEU	466	22.156	18.002	-7.482	1.00	48.32
	ATOM	1264	CD2	LEU	466	22.033	18.594	-5.057	1.00	48.14
	ATOM	1265	C	LEU	466	23.817	16.397	-3.650	1.00	48.16
30	ATOM	1266	O	LEU	466	22.961	16.845	-2.883	1.00	45.90
	ATOM	1267	N	LYS	467	24.093	15.099	-3.750	1.00	46.47
	ATOM	1268	CA	LYS	467	23.399	14.100	-2.947	1.00	47.45
	ATOM	1269	CB	LYS	467	23.802	12.693	-3.395	1.00	49.38
	ATOM	1270	CG	LYS	467	22.829	11.602	-2.974	1.00	52.70
35	ATOM	1271	CD	LYS	467	23.561	10.301	-2.682	1.00	56.48
	ATOM	1272	CE	LYS	467	23.105	9.180	-3.604	1.00	59.54
	ATOM	1273	NZ	LYS	467	24.150	8.117	-3.732	1.00	61.22
	ATOM	1274	C	LYS	467	23.738	14.284	-1.472	1.00	46.89
	ATOM	1275	O	LYS	467	22.884	14.108	-0.604	1.00	46.06
40	ATOM	1276	N	SER	468	24.989	14.644	-1.202	1.00	45.82
	ATOM	1277	CA	SER	468	25.457	14.854	0.160	1.00	46.82
	ATOM	1278	CB	SER	468	26.976	15.050	0.173	1.00	47.85
	ATOM	1279	OG	SER	468	27.407	15.537	1.435	1.00	55.73
	ATOM	1280	C	SER	468	24.778	16.063	0.790	1.00	44.24
45	ATOM	1281	O	SER	468	24.473	16.062	1.983	1.00	42.98
	ATOM	1282	N	LEU	469	24.547	17.100	-0.011	1.00	42.33
	ATOM	1283	CA	LEU	469	23.890	18.301	0.486	1.00	40.42
	ATOM	1284	CB	LEU	469	24.002	19.427	-0.545	1.00	44.47
	ATOM	1285	CG	LEU	469	25.438	19.874	-0.849	1.00	46.70
50	ATOM	1286	CD1	LEU	469	25.514	20.477	-2.246	1.00	46.70
	ATOM	1287	CD2	LEU	469	25.890	20.883	0.199	1.00	47.32
	ATOM	1288	C	LEU	469	22.423	17.996	0.786	1.00	39.06
	ATOM	1289	O	LEU	469	21.856	18.505	1.760	1.00	34.97
	ATOM	1290	N	GLU	470	21.814	17.151	-0.046	1.00	35.46
55	ATOM	1291	CA	GLU	470	20.418	16.768	0.145	1.00	34.38
	ATOM	1292	CB	GLU	470	19.914	15.963	-1.052	1.00	38.02
	ATOM	1293	CG	GLU	470	19.772	16.773	-2.329	1.00	42.67
	ATOM	1294	CD	GLU	470	19.339	15.923	-3.509	1.00	48.30
	ATOM	1295	OE1	GLU	470	19.671	14.716	-3.538	1.00	50.53
60	ATOM	1296	OE2	GLU	470	18.666	16.463	-4.412	1.00	51.06
	ATOM	1297	C	GLU	470	20.290	15.916	1.403	1.00	34.37



5	ATOM	1298	O	GLU	470	19.321	16.035	2.157	1.00	32.60
	ATOM	1299	N	GLU	471	21.274	15.046	1.606	1.00	34.66
	ATOM	1300	CA	GLU	471	21.309	14.162	2.766	1.00	35.68
	ATOM	1301	CB	GLU	471	22.515	13.222	2.671	1.00	34.57
	ATOM	1302	CG	GLU	471	22.376	12.122	1.614	1.00	37.98
10	ATOM	1303	CD	GLU	471	21.476	10.989	2.063	1.00	39.79
	ATOM	1304	OE1	GLU	471	20.268	11.027	1.743	1.00	41.12
	ATOM	1305	OE2	GLU	471	21.974	10.061	2.737	1.00	32.11
	ATOM	1306	C	GLU	471	21.393	14.983	4.052	1.00	34.79
	ATOM	1307	O	GLU	471	20.596	14.793	4.969	1.00	32.80
15	ATOM	1308	N	LYS	472	22.358	15.898	4.112	1.00	33.93
	ATOM	1309	CA	LYS	472	22.518	16.739	5.291	1.00	35.58
	ATOM	1310	CB	LYS	472	23.683	17.710	5.097	1.00	39.11
	ATOM	1311	CG	LYS	472	25.050	17.050	5.138	1.00	41.47
	ATOM	1312	CD	LYS	472	26.080	17.957	5.794	1.00	46.97
20	ATOM	1313	CE	LYS	472	27.445	17.286	5.862	1.00	48.40
	ATOM	1314	NZ	LYS	472	27.850	16.702	4.547	1.00	51.55
	ATOM	1315	C	LYS	472	21.237	17.523	5.582	1.00	34.78
	ATOM	1316	O	LYS	472	20.795	17.607	6.724	1.00	33.95
	ATOM	1317	N	ASP	473	20.643	18.097	4.545	1.00	33.47
25	ATOM	1318	CA	ASP	473	19.420	18.865	4.720	1.00	34.63
	ATOM	1319	CB	ASP	473	18.923	19.404	3.380	1.00	37.21
	ATOM	1320	CG	ASP	473	17.654	20.221	3.522	1.00	43.24
	ATOM	1321	OD1	ASP	473	16.559	19.687	3.230	1.00	45.20
	ATOM	1322	OD2	ASP	473	17.750	21.396	3.932	1.00	45.59
30	ATOM	1323	C	ASP	473	18.339	17.998	5.338	1.00	32.93
	ATOM	1324	O	ASP	473	17.642	18.416	6.264	1.00	32.87
	ATOM	1325	N	HIS	474	18.199	16.784	4.827	1.00	32.74
	ATOM	1326	CA	HIS	474	17.185	15.882	5.343	1.00	32.21
	ATOM	1327	CB	HIS	474	17.185	14.575	4.568	1.00	32.79
35	ATOM	1328	CG	HIS	474	16.047	13.675	4.924	1.00	36.22
	ATOM	1329	CD2	HIS	474	14.711	13.813	4.750	1.00	38.33
	ATOM	1330	ND1	HIS	474	16.227	12.456	5.542	1.00	38.97
	ATOM	1331	CE1	HIS	474	15.053	11.883	5.732	1.00	37.99
	ATOM	1332	NE2	HIS	474	14.116	12.686	5.261	1.00	37.43
40	ATOM	1333	C	HIS	474	17.403	15.573	6.815	1.00	29.74
	ATOM	1334	O	HIS	474	16.460	15.543	7.596	1.00	29.90
	ATOM	1335	N	ILE	475	18.653	15.326	7.185	1.00	27.80
	ATOM	1336	CA	ILE	475	18.971	15.014	8.571	1.00	25.61
	ATOM	1337	CB	ILE	475	20.478	14.708	8.720	1.00	25.59
45	ATOM	1338	CG2	ILE	475	20.877	14.713	10.193	1.00	27.17
	ATOM	1339	CG1	ILE	475	20.787	13.341	8.092	1.00	26.17
	ATOM	1340	CD1	ILE	475	22.258	13.071	7.849	1.00	27.07
	ATOM	1341	C	ILE	475	18.576	16.201	9.460	1.00	27.91
	ATOM	1342	O	ILE	475	17.928	16.038	10.485	1.00	29.16
50	ATOM	1343	N	HIS	476	18.956	17.404	9.054	1.00	29.41
	ATOM	1344	CA	HIS	476	18.621	18.575	9.846	1.00	29.73
	ATOM	1345	CB	HIS	476	19.342	19.796	9.281	1.00	32.27
	ATOM	1346	CG	HIS	476	20.777	19.867	9.699	1.00	39.44
	ATOM	1347	CD2	HIS	476	21.355	19.707	10.915	1.00	39.81
55	ATOM	1348	ND1	HIS	476	21.809	20.067	8.808	1.00	39.79
	ATOM	1349	CE1	HIS	476	22.959	20.027	9.456	1.00	39.98
	ATOM	1350	NE2	HIS	476	22.712	19.809	10.735	1.00	40.26
	ATOM	1351	C	HIS	476	17.120	18.810	9.948	1.00	31.40
	ATOM	1352	O	HIS	476	16.636	19.336	10.951	1.00	29.79
60	ATOM	1353	N	ARG	477	16.374	18.396	8.929	1.00	31.82
	ATOM	1354	CA	ARG	477	14.929	18.570	8.956	1.00	31.53

5	ATOM	1355	CB	ARG	477	14.343	18.376	7.557	1.00	34.95
	ATOM	1356	CG	ARG	477	14.425	19.627	6.700	1.00	40.46
	ATOM	1357	CD	ARG	477	13.698	19.445	5.370	1.00	45.22
	ATOM	1358	NE	ARG	477	14.107	20.456	4.399	1.00	53.05
	ATOM	1359	CZ	ARG	477	13.647	21.705	4.376	1.00	55.89
10	ATOM	1360	NH1	ARG	477	12.756	22.106	5.274	1.00	56.17
	ATOM	1361	NH2	ARG	477	14.084	22.558	3.457	1.00	59.49
	ATOM	1362	C	ARG	477	14.310	17.582	9.931	1.00	30.70
	ATOM	1363	O	ARG	477	13.360	17.903	10.649	1.00	30.24
	ATOM	1364	N	VAL	478	14.863	16.375	9.972	1.00	29.67
15	ATOM	1365	CA	VAL	478	14.351	15.369	10.887	1.00	29.68
	ATOM	1366	CB	VAL	478	14.937	13.975	10.575	1.00	32.01
	ATOM	1367	CG1	VAL	478	14.461	12.973	11.609	1.00	32.93
	ATOM	1368	CG2	VAL	478	14.506	13.528	9.169	1.00	31.00
	ATOM	1369	C	VAL	478	14.696	15.774	12.316	1.00	29.81
20	ATOM	1370	O	VAL	478	13.860	15.677	13.220	1.00	30.25
	ATOM	1371	N	LEU	479	15.929	16.232	12.516	1.00	28.81
	ATOM	1372	CA	LEU	479	16.360	16.674	13.836	1.00	28.74
	ATOM	1373	CB	LEU	479	17.799	17.210	13.779	1.00	26.65
	ATOM	1374	CG	LEU	479	18.910	16.152	13.853	1.00	26.05
25	ATOM	1375	CD1	LEU	479	20.231	16.772	13.395	1.00	25.81
	ATOM	1376	CD2	LEU	479	19.028	15.603	15.277	1.00	25.34
	ATOM	1377	C	LEU	479	15.411	17.777	14.313	1.00	29.54
	ATOM	1378	O	LEU	479	14.997	17.786	15.472	1.00	29.00
	ATOM	1379	N	ASP	480	15.076	18.703	13.415	1.00	31.52
30	ATOM	1380	CA	ASP	480	14.162	19.800	13.741	1.00	33.84
	ATOM	1381	CB	ASP	480	13.943	20.712	12.528	1.00	34.37
	ATOM	1382	CG	ASP	480	15.055	21.743	12.345	1.00	36.26
	ATOM	1383	OD1	ASP	480	15.119	22.354	11.257	1.00	36.56
	ATOM	1384	OD2	ASP	480	15.860	21.951	13.274	1.00	34.19
35	ATOM	1385	C	ASP	480	12.818	19.222	14.174	1.00	33.48
	ATOM	1386	O	ASP	480	12.186	19.724	15.105	1.00	33.89
	ATOM	1387	N	LYS	481	12.379	18.161	13.498	1.00	33.90
	ATOM	1388	CA	LYS	481	11.106	17.536	13.839	1.00	32.97
	ATOM	1389	CB	LYS	481	10.719	16.489	12.784	1.00	34.66
40	ATOM	1390	C	LYS	481	11.164	16.895	15.225	1.00	33.57
	ATOM	1391	O	LYS	481	10.167	16.869	15.943	1.00	35.37
	ATOM	1392	N	ILE	482	12.328	16.377	15.607	1.00	32.71
	ATOM	1393	CA	ILE	482	12.457	15.764	16.922	1.00	31.60
	ATOM	1394	CB	ILE	482	13.743	14.913	17.028	1.00	32.65
45	ATOM	1395	CG2	ILE	482	13.877	14.338	18.430	1.00	32.50
	ATOM	1396	CG1	ILE	482	13.697	13.785	15.995	1.00	32.72
	ATOM	1397	CD1	ILE	482	14.978	12.969	15.908	1.00	33.37
	ATOM	1398	C	ILE	482	12.456	16.853	17.994	1.00	31.69
	ATOM	1399	O	ILE	482	11.946	16.649	19.097	1.00	29.98
50	ATOM	1400	N	THR	483	13.027	18.012	17.679	1.00	31.33
	ATOM	1401	CA	THR	483	13.022	19.109	18.644	1.00	31.71
	ATOM	1402	CB	THR	483	13.756	20.351	18.109	1.00	32.92
	ATOM	1403	OG1	THR	483	15.111	20.012	17.788	1.00	29.99
	ATOM	1404	CG2	THR	483	13.756	21.452	19.160	1.00	30.47
55	ATOM	1405	C	THR	483	11.559	19.483	18.920	1.00	32.85
	ATOM	1406	O	THR	483	11.146	19.598	20.070	1.00	31.83
	ATOM	1407	N	ASP	484	10.785	19.656	17.851	1.00	31.91
	ATOM	1408	CA	ASP	484	9.369	20.003	17.965	1.00	34.15
	ATOM	1409	CB	ASP	484	8.708	20.013	16.591	1.00	37.41
60	ATOM	1410	CG	ASP	484	9.270	21.080	15.680	1.00	42.02
	ATOM	1411	OD1	ASP	484	9.871	22.045	16.198	1.00	43.26

5	ATOM	1412	OD2	ASP	484	9.106	20.952	14.445	1.00	42.49
	ATOM	1413	C	ASP	484	8.657	18.985	18.840	1.00	33.16
	ATOM	1414	O	ASP	484	7.830	19.339	19.676	1.00	34.86
	ATOM	1415	N	THR	485	8.996	17.715	18.646	1.00	33.91
	ATOM	1416	CA	THR	485	8.396	16.635	19.414	1.00	34.41
10	ATOM	1417	CB	THR	485	8.875	15.268	18.885	1.00	33.58
	ATOM	1418	OG1	THR	485	8.400	15.094	17.542	1.00	37.04
	ATOM	1419	CG2	THR	485	8.347	14.138	19.751	1.00	30.89
	ATOM	1420	C	THR	485	8.708	16.757	20.903	1.00	35.15
	ATOM	1421	O	THR	485	7.818	16.600	21.744	1.00	31.99
15	ATOM	1422	N	LEU	486	9.966	17.046	21.229	1.00	33.77
	ATOM	1423	CA	LEU	486	10.368	17.192	22.621	1.00	34.31
	ATOM	1424	CB	LEU	486	11.879	17.448	22.721	1.00	32.00
	ATOM	1425	CG	LEU	486	12.776	16.201	22.754	1.00	34.99
	ATOM	1426	CD1	LEU	486	14.233	16.613	22.521	1.00	32.65
20	ATOM	1427	CD2	LEU	486	12.635	15.481	24.105	1.00	29.90
	ATOM	1428	C	LEU	486	9.597	18.348	23.256	1.00	34.87
	ATOM	1429	O	LEU	486	9.078	18.225	24.362	1.00	35.85
	ATOM	1430	N	ILE	487	9.513	19.469	22.548	1.00	35.59
	ATOM	1431	CA	ILE	487	8.787	20.625	23.064	1.00	36.79
25	ATOM	1432	CB	ILE	487	8.890	21.826	22.095	1.00	37.32
	ATOM	1433	CG2	ILE	487	7.833	22.884	22.443	1.00	40.19
	ATOM	1434	CG1	ILE	487	10.292	22.443	22.181	1.00	36.00
	ATOM	1435	CD1	ILE	487	10.635	23.041	23.544	1.00	33.58
	ATOM	1436	C	ILE	487	7.315	20.257	23.276	1.00	38.56
30	ATOM	1437	O	ILE	487	6.708	20.628	24.282	1.00	38.52
	ATOM	1438	N	HIS	488	6.749	19.521	22.326	1.00	40.33
	ATOM	1439	CA	HIS	488	5.357	19.096	22.427	1.00	42.29
	ATOM	1440	CB	HIS	488	4.962	18.282	21.197	1.00	44.26
	ATOM	1441	CG	HIS	488	3.612	17.647	21.305	1.00	47.75
35	ATOM	1442	CD2	HIS	488	2.369	18.175	21.214	1.00	47.46
	ATOM	1443	ND1	HIS	488	3.440	16.298	21.534	1.00	51.09
	ATOM	1444	CE1	HIS	488	2.148	16.023	21.577	1.00	51.15
	ATOM	1445	NE2	HIS	488	1.477	17.144	21.385	1.00	50.22
	ATOM	1446	C	HIS	488	5.154	18.254	23.685	1.00	42.55
40	ATOM	1447	O	HIS	488	4.233	18.498	24.467	1.00	43.02
	ATOM	1448	N	LEU	489	6.022	17.266	23.879	1.00	39.91
	ATOM	1449	CA	LEU	489	5.936	16.399	25.048	1.00	39.93
	ATOM	1450	CB	LEU	489	7.087	15.396	25.048	1.00	38.83
	ATOM	1451	CG	LEU	489	6.961	14.242	24.056	1.00	39.31
45	ATOM	1452	CD1	LEU	489	8.259	13.456	24.027	1.00	39.01
	ATOM	1453	CD2	LEU	489	5.799	13.345	24.459	1.00	41.98
	ATOM	1454	C	LEU	489	5.973	17.203	26.339	1.00	40.24
	ATOM	1455	O	LEU	489	5.267	16.888	27.298	1.00	38.72
	ATOM	1456	N	MET	490	6.798	18.246	26.353	1.00	39.94
50	ATOM	1457	CA	MET	490	6.939	19.102	27.522	1.00	41.50
	ATOM	1458	CB	MET	490	8.208	19.953	27.394	1.00	39.15
	ATOM	1459	CG	MET	490	9.495	19.169	27.608	1.00	41.69
	ATOM	1460	SD	MET	490	10.978	20.106	27.161	1.00	35.76
	ATOM	1461	CE	MET	490	12.178	18.775	27.056	1.00	39.22
55	ATOM	1462	C	MET	490	5.718	20.004	27.717	1.00	42.33
	ATOM	1463	O	MET	490	5.296	20.258	28.848	1.00	41.09
	ATOM	1464	N	ALA	491	5.162	20.498	26.616	1.00	43.15
	ATOM	1465	CA	ALA	491	3.983	21.351	26.693	1.00	43.79
	ATOM	1466	CB	ALA	491	3.622	21.879	25.311	1.00	43.93
60	ATOM	1467	C	ALA	491	2.841	20.510	27.251	1.00	46.16
	ATOM	1468	O	ALA	491	2.073	20.967	28.095	1.00	44.69

5	ATOM	1469	N	LYS	492	2.752	19.268	26.783	1.00	46.29
	ATOM	1470	CA	LYS	492	1.711	18.351	27.222	1.00	49.90
	ATOM	1471	CB	LYS	492	1.772	17.053	26.411	1.00	50.03
	ATOM	1472	CG	LYS	492	1.087	17.135	25.062	1.00	53.81
	ATOM	1473	CD	LYS	492	-0.002	16.084	24.930	1.00	59.00
10	ATOM	1474	CE	LYS	492	-0.988	16.453	23.827	1.00	61.85
	ATOM	1475	NZ	LYS	492	-1.351	15.281	22.976	1.00	62.89
	ATOM	1476	C	LYS	492	1.841	18.025	28.701	1.00	51.15
	ATOM	1477	O	LYS	492	0.845	17.784	29.379	1.00	53.37
	ATOM	1478	N	ALA	493	3.072	18.012	29.199	1.00	50.15
15	ATOM	1479	CA	ALA	493	3.321	17.706	30.600	1.00	49.17
	ATOM	1480	CB	ALA	493	4.777	17.314	30.794	1.00	50.39
	ATOM	1481	C	ALA	493	2.971	18.885	31.501	1.00	49.36
	ATOM	1482	O	ALA	493	3.089	18.799	32.723	1.00	51.57
	ATOM	1483	N	GLY	494	2.554	19.989	30.893	1.00	48.61
20	ATOM	1484	CA	GLY	494	2.185	21.159	31.671	1.00	46.92
	ATOM	1485	C	GLY	494	3.322	22.107	32.006	1.00	45.46
	ATOM	1486	O	GLY	494	3.206	22.921	32.919	1.00	43.58
	ATOM	1487	N	LEU	495	4.431	22.009	31.284	1.00	44.81
	ATOM	1488	CA	LEU	495	5.555	22.899	31.540	1.00	42.34
25	ATOM	1489	CB	LEU	495	6.847	22.293	30.988	1.00	43.79
	ATOM	1490	CG	LEU	495	7.712	21.459	31.936	1.00	40.99
	ATOM	1491	CD1	LEU	495	7.022	20.156	32.260	1.00	44.70
	ATOM	1492	CD2	LEU	495	9.072	21.189	31.270	1.00	42.12
	ATOM	1493	C	LEU	495	5.278	24.227	30.847	1.00	42.13
30	ATOM	1494	O	LEU	495	4.664	24.258	29.778	1.00	42.49
	ATOM	1495	N	THR	496	5.718	25.324	31.452	1.00	42.73
	ATOM	1496	CA	THR	496	5.521	26.636	30.845	1.00	43.56
	ATOM	1497	CB	THR	496	5.841	27.767	31.829	1.00	46.09
	ATOM	1498	OG1	THR	496	7.222	27.688	32.208	1.00	43.92
35	ATOM	1499	CG2	THR	496	4.965	27.662	33.064	1.00	45.63
	ATOM	1500	C	THR	496	6.471	26.764	29.660	1.00	45.54
	ATOM	1501	O	THR	496	7.370	25.939	29.488	1.00	43.39
	ATOM	1502	N	LEU	497	6.280	27.800	28.849	1.00	45.02
	ATOM	1503	CA	LEU	497	7.135	28.020	27.688	1.00	45.12
40	ATOM	1504	CB	LEU	497	6.710	29.286	26.944	1.00	46.62
	ATOM	1505	CG	LEU	497	5.933	29.080	25.640	1.00	50.20
	ATOM	1506	CD1	LEU	497	5.886	30.397	24.875	1.00	50.95
	ATOM	1507	CD2	LEU	497	6.589	27.990	24.798	1.00	50.91
	ATOM	1508	C	LEU	497	8.599	28.135	28.101	1.00	44.94
45	ATOM	1509	O	LEU	497	9.474	27.516	27.493	1.00	45.03
	ATOM	1510	N	GLN	498	8.862	28.927	29.137	1.00	41.14
	ATOM	1511	CA	GLN	498	10.221	29.101	29.627	1.00	40.54
	ATOM	1512	CB	GLN	498	10.246	30.140	30.743	1.00	43.82
	ATOM	1513	CG	GLN	498	11.585	30.270	31.437	1.00	43.37
50	ATOM	1514	CD	GLN	498	11.539	31.260	32.584	1.00	47.03
	ATOM	1515	OE1	GLN	498	10.565	31.308	33.332	1.00	49.18
	ATOM	1516	NE2	GLN	498	12.591	32.054	32.727	1.00	45.30
	ATOM	1517	C	GLN	498	10.777	27.773	30.145	1.00	39.39
	ATOM	1518	O	GLN	498	11.923	27.422	29.866	1.00	35.05
55	ATOM	1519	N	GLN	499	9.965	27.040	30.902	1.00	36.49
	ATOM	1520	CA	GLN	499	10.391	25.748	31.434	1.00	36.91
	ATOM	1521	CB	GLN	499	9.314	25.155	32.344	1.00	38.84
	ATOM	1522	CG	GLN	499	9.155	25.825	33.703	1.00	41.33
	ATOM	1523	CD	GLN	499	8.039	25.187	34.512	1.00	42.74
60	ATOM	1524	OE1	GLN	499	7.027	24.760	33.955	1.00	45.44
	ATOM	1525	NE2	GLN	499	8.222	25.107	35.829	1.00	43.48

5	ATOM	1526	C	GLN	499	10.655	24.773	30.285	1.00	35.03
	ATOM	1527	O	GLN	499	11.446	23.832	30.422	1.00	36.59
	ATOM	1528	N	GLN	500	9.980	24.994	29.162	1.00	34.14
	ATOM	1529	CA	GLN	500	10.136	24.138	27.990	1.00	34.65
	ATOM	1530	CB	GLN	500	9.042	24.436	26.958	1.00	33.90
10	ATOM	1531	CG	GLN	500	7.672	23.872	27.315	1.00	36.62
	ATOM	1532	CD	GLN	500	6.558	24.419	26.435	1.00	40.17
	ATOM	1533	OE1	GLN	500	6.660	24.417	25.207	1.00	40.22
	ATOM	1534	NE2	GLN	500	5.482	24.886	27.064	1.00	41.82
	ATOM	1535	C	GLN	500	11.511	24.350	27.358	1.00	34.96
15	ATOM	1536	O	GLN	500	12.256	23.387	27.124	1.00	30.79
	ATOM	1537	N	HIS	501	11.835	25.612	27.078	1.00	34.21
	ATOM	1538	CA	HIS	501	13.117	25.966	26.480	1.00	37.42
	ATOM	1539	CB	HIS	501	13.195	27.476	26.246	1.00	43.08
	ATOM	1540	CG	HIS	501	12.043	28.027	25.468	1.00	51.13
20	ATOM	1541	CD2	HIS	501	11.534	27.678	24.263	1.00	53.05
	ATOM	1542	ND1	HIS	501	11.264	29.068	25.926	1.00	54.54
	ATOM	1543	CE1	HIS	501	10.325	29.337	25.037	1.00	54.36
	ATOM	1544	NE2	HIS	501	10.466	28.508	24.018	1.00	55.19
	ATOM	1545	C	HIS	501	14.255	25.543	27.395	1.00	35.79
25	ATOM	1546	O	HIS	501	15.271	24.996	26.945	1.00	36.20
	ATOM	1547	N	GLN	502	14.086	25.799	28.685	1.00	33.90
	ATOM	1548	CA	GLN	502	15.110	25.438	29.650	1.00	32.18
	ATOM	1549	CB	GLN	502	14.740	25.977	31.033	1.00	35.84
	ATOM	1550	CG	GLN	502	14.787	27.498	31.113	1.00	32.66
30	ATOM	1551	CD	GLN	502	14.420	28.028	32.486	1.00	36.62
	ATOM	1552	OE1	GLN	502	14.102	27.262	33.397	1.00	33.99
	ATOM	1553	NE2	GLN	502	14.462	29.348	32.640	1.00	36.22
	ATOM	1554	C	GLN	502	15.340	23.932	29.716	1.00	31.79
	ATOM	1555	O	GLN	502	16.483	23.479	29.769	1.00	28.00
35	ATOM	1556	N	ARG	503	14.266	23.146	29.705	1.00	30.99
	ATOM	1557	CA	ARG	503	14.436	21.704	29.779	1.00	29.91
	ATOM	1558	CB	ARG	503	13.107	21.011	30.052	1.00	32.79
	ATOM	1559	CG	ARG	503	13.258	19.541	30.400	1.00	30.84
	ATOM	1560	CD	ARG	503	11.930	18.935	30.798	1.00	30.61
40	ATOM	1561	NE	ARG	503	12.021	17.490	30.992	1.00	28.50
	ATOM	1562	CZ	ARG	503	12.489	16.908	32.093	1.00	29.00
	ATOM	1563	NH1	ARG	503	12.917	17.640	33.114	1.00	29.85
	ATOM	1564	NH2	ARG	503	12.512	15.583	32.180	1.00	33.73
	ATOM	1565	C	ARG	503	15.051	21.152	28.496	1.00	29.89
45	ATOM	1566	O	ARG	503	15.895	20.259	28.548	1.00	29.69
	ATOM	1567	N	LEU	504	14.624	21.675	27.351	1.00	28.99
	ATOM	1568	CA	LEU	504	15.164	21.223	26.075	1.00	28.90
	ATOM	1569	CB	LEU	504	14.566	22.023	24.916	1.00	27.72
	ATOM	1570	CG	LEU	504	15.327	21.901	23.593	1.00	30.47
50	ATOM	1571	CD1	LEU	504	15.252	20.453	23.117	1.00	31.74
	ATOM	1572	CD2	LEU	504	14.742	22.843	22.542	1.00	29.85
	ATOM	1573	C	LEU	504	16.681	21.419	26.089	1.00	29.69
	ATOM	1574	O	LEU	504	17.439	20.536	25.672	1.00	26.38
	ATOM	1575	N	ALA	505	17.114	22.585	26.564	1.00	28.51
55	ATOM	1576	CA	ALA	505	18.535	22.899	26.632	1.00	25.98
	ATOM	1577	CB	ALA	505	18.735	24.361	27.039	1.00	29.86
	ATOM	1578	C	ALA	505	19.261	21.977	27.604	1.00	26.67
	ATOM	1579	O	ALA	505	20.340	21.462	27.290	1.00	25.54
	ATOM	1580	N	GLN	506	18.677	21.771	28.784	1.00	23.59
60	ATOM	1581	CA	GLN	506	19.299	20.907	29.785	1.00	27.67
	ATOM	1582	CB	GLN	506	18.434	20.796	31.043	1.00	27.75

5	ATOM	1583	CG	GLN	506	18.414	22.027	31.945	1.00	32.48
	ATOM	1584	CD	GLN	506	17.111	22.116	32.736	1.00	38.40
	ATOM	1585	OE1	GLN	506	16.319	21.167	32.754	1.00	35.97
	ATOM	1586	NE2	GLN	506	16.879	23.257	33.386	1.00	38.07
	ATOM	1587	C	GLN	506	19.500	19.509	29.217	1.00	24.53
10	ATOM	1588	O	GLN	506	20.536	18.889	29.441	1.00	26.42
	ATOM	1589	N	LEU	507	18.505	19.017	28.484	1.00	26.78
	ATOM	1590	CA	LEU	507	18.578	17.678	27.902	1.00	26.18
	ATOM	1591	CB	LEU	507	17.225	17.286	27.295	1.00	31.48
	ATOM	1592	CG	LEU	507	16.052	16.961	28.231	1.00	32.59
15	ATOM	1593	CD1	LEU	507	14.836	16.561	27.389	1.00	33.78
	ATOM	1594	CD2	LEU	507	16.431	15.838	29.174	1.00	30.18
	ATOM	1595	C	LEU	507	19.652	17.583	26.819	1.00	26.03
	ATOM	1596	O	LEU	507	20.421	16.621	26.771	1.00	27.28
	ATOM	1597	N	LEU	508	19.713	18.583	25.950	1.00	24.31
20	ATOM	1598	CA	LEU	508	20.690	18.557	24.863	1.00	23.68
	ATOM	1599	CB	LEU	508	20.339	19.629	23.828	1.00	23.91
	ATOM	1600	CG	LEU	508	19.004	19.436	23.102	1.00	24.68
	ATOM	1601	CD1	LEU	508	18.905	20.416	21.945	1.00	25.11
	ATOM	1602	CD2	LEU	508	18.903	17.994	22.580	1.00	27.53
25	ATOM	1603	C	LEU	508	22.127	18.727	25.341	1.00	22.93
	ATOM	1604	O	LEU	508	23.062	18.200	24.736	1.00	21.36
	ATOM	1605	N	LEU	509	22.302	19.451	26.441	1.00	23.86
	ATOM	1606	CA	LEU	509	23.637	19.661	26.991	1.00	26.28
	ATOM	1607	CB	LEU	509	23.598	20.735	28.095	1.00	28.08
30	ATOM	1608	CG	LEU	509	23.578	22.214	27.672	1.00	33.98
	ATOM	1609	CD1	LEU	509	23.529	23.114	28.921	1.00	35.23
	ATOM	1610	CD2	LEU	509	24.818	22.525	26.856	1.00	30.48
	ATOM	1611	C	LEU	509	24.154	18.327	27.540	1.00	26.08
	ATOM	1612	O	LEU	509	25.354	18.068	27.547	1.00	23.92
35	ATOM	1613	N	ILE	510	23.254	17.462	27.993	1.00	24.60
	ATOM	1614	CA	ILE	510	23.712	16.172	28.496	1.00	25.12
	ATOM	1615	CB	ILE	510	22.568	15.368	29.161	1.00	28.51
	ATOM	1616	CG2	ILE	510	23.051	13.965	29.506	1.00	31.67
	ATOM	1617	CG1	ILE	510	22.141	16.060	30.459	1.00	31.18
40	ATOM	1618	CD1	ILE	510	20.712	15.749	30.882	1.00	37.16
	ATOM	1619	C	ILE	510	24.337	15.351	27.364	1.00	23.86
	ATOM	1620	O	ILE	510	25.225	14.534	27.600	1.00	24.14
	ATOM	1621	N	LEU	511	23.889	15.586	26.133	1.00	25.10
	ATOM	1622	CA	LEU	511	24.420	14.862	24.977	1.00	25.63
45	ATOM	1623	CB	LEU	511	23.628	15.225	23.714	1.00	23.89
	ATOM	1624	CG	LEU	511	22.152	14.801	23.659	1.00	25.78
	ATOM	1625	CD1	LEU	511	21.648	14.920	22.224	1.00	26.55
	ATOM	1626	CD2	LEU	511	21.990	13.363	24.146	1.00	26.29
	ATOM	1627	C	LEU	511	25.912	15.152	24.771	1.00	27.10
50	ATOM	1628	O	LEU	511	26.641	14.332	24.214	1.00	24.98
	ATOM	1629	N	SER	512	26.372	16.319	25.213	1.00	24.75
	ATOM	1630	CA	SER	512	27.787	16.637	25.076	1.00	23.68
	ATOM	1631	CB	SER	512	28.023	18.129	25.358	1.00	26.12
	ATOM	1632	OG	SER	512	29.271	18.327	25.986	1.00	37.17
55	ATOM	1633	C	SER	512	28.594	15.765	26.050	1.00	23.15
	ATOM	1634	O	SER	512	29.742	15.383	25.769	1.00	22.15
	ATOM	1635	N	AHIS	513	27.993	15.456	27.192	0.50	21.53
	ATOM	1636	N	BHIS	513	28.008	15.453	27.202	0.50	20.99
	ATOM	1637	CA	AHIS	513	28.645	14.624	28.196	0.50	21.79
60	ATOM	1638	CA	BHIS	513	28.696	14.607	28.174	0.50	20.94
	ATOM	1639	CB	AHIS	513	27.920	14.776	29.536	0.50	23.59

5	ATOM	1640	CB	BHIS	513	27.991	14.636	29.536	0.50	21.59
	ATOM	1641	CG	AHIS	513	28.145	16.109	30.179	0.50	27.34
	ATOM	1642	CG	BHIS	513	28.800	14.032	30.642	0.50	23.94
	ATOM	1643	CD2	AHIS	513	29.223	16.616	30.824	0.50	27.56
	ATOM	1644	CD2	BHIS	513	30.095	14.211	31.001	0.50	24.22
10	ATOM	1645	ND1	AHIS	513	27.204	17.117	30.160	0.50	30.62
	ATOM	1646	ND1	BHIS	513	28.285	13.105	31.523	0.50	27.00
	ATOM	1647	CE1	AHIS	513	27.693	18.185	30.763	0.50	26.32
	ATOM	1648	CE1	BHIS	513	29.225	12.740	32.376	0.50	24.40
	ATOM	1649	NE2	AHIS	513	28.916	17.908	31.176	0.50	28.30
15	ATOM	1650	NE2	BHIS	513	30.334	13.396	32.081	0.50	25.54
	ATOM	1651	C	AHIS	513	28.666	13.164	27.738	0.50	19.81
	ATOM	1652	C	BHIS	513	28.720	13.171	27.652	0.50	19.42
	ATOM	1653	O	AHIS	513	29.601	12.426	28.026	0.50	22.45
	ATOM	1654	O	BHIS	513	29.707	12.457	27.809	0.50	22.62
20	ATOM	1655	N	ILE	514	27.633	12.753	27.015	1.00	20.76
	ATOM	1656	CA	ILE	514	27.572	11.396	26.492	1.00	20.94
	ATOM	1657	CB	ILE	514	26.154	11.086	25.953	1.00	27.76
	ATOM	1658	CG2	ILE	514	26.169	9.800	25.123	1.00	28.26
	ATOM	1659	CG1	ILE	514	25.185	10.965	27.139	1.00	27.91
25	ATOM	1660	CD1	ILE	514	23.752	10.649	26.753	1.00	34.31
	ATOM	1661	C	ILE	514	28.641	11.256	25.398	1.00	20.66
	ATOM	1662	O	ILE	514	29.298	10.226	25.285	1.00	22.21
	ATOM	1663	N	ARG	515	28.825	12.294	24.589	1.00	20.48
	ATOM	1664	CA	ARG	515	29.861	12.243	23.554	1.00	21.98
30	ATOM	1665	CB	ARG	515	29.861	13.535	22.726	1.00	23.11
	ATOM	1666	CG	ARG	515	31.003	13.611	21.737	1.00	25.76
	ATOM	1667	CD	ARG	515	30.664	12.818	20.491	1.00	28.55
	ATOM	1668	NE	ARG	515	29.580	13.482	19.788	1.00	36.24
	ATOM	1669	CZ	ARG	515	29.615	13.827	18.508	1.00	38.91
35	ATOM	1670	NH1	ARG	515	30.689	13.566	17.776	1.00	35.37
	ATOM	1671	NH2	ARG	515	28.579	14.459	17.971	1.00	40.27
	ATOM	1672	C	ARG	515	31.221	12.087	24.225	1.00	21.29
	ATOM	1673	O	ARG	515	32.068	11.305	23.795	1.00	20.06
	ATOM	1674	N	HIS	516	31.420	12.844	25.293	1.00	23.23
40	ATOM	1675	CA	HIS	516	32.675	12.812	26.034	1.00	24.75
	ATOM	1676	CB	HIS	516	32.566	13.794	27.206	1.00	24.03
	ATOM	1677	CG	HIS	516	33.826	13.948	27.990	1.00	31.42
	ATOM	1678	CD2	HIS	516	34.138	13.587	29.257	1.00	35.87
	ATOM	1679	ND1	HIS	516	34.938	14.586	27.489	1.00	33.59
45	ATOM	1680	CE1	HIS	516	35.882	14.613	28.411	1.00	35.70
	ATOM	1681	NE2	HIS	516	35.422	14.013	29.495	1.00	33.35
	ATOM	1682	C	HIS	516	32.965	11.390	26.537	1.00	24.02
	ATOM	1683	O	HIS	516	34.059	10.852	26.362	1.00	23.66
	ATOM	1684	N	MET	517	31.969	10.786	27.168	1.00	20.91
50	ATOM	1685	CA	MET	517	32.109	9.436	27.684	1.00	24.21
	ATOM	1686	CB	MET	517	30.837	9.038	28.424	1.00	23.88
	ATOM	1687	CG	MET	517	30.607	9.903	29.652	1.00	26.32
	ATOM	1688	SD	MET	517	29.435	9.222	30.790	1.00	26.67
	ATOM	1689	CE	MET	517	27.914	9.390	29.807	1.00	23.26
55	ATOM	1690	C	MET	517	32.399	8.448	26.564	1.00	23.26
	ATOM	1691	O	MET	517	33.213	7.547	26.728	1.00	26.08
	ATOM	1692	N	SER	518	31.736	8.612	25.423	1.00	21.93
	ATOM	1693	CA	SER	518	31.977	7.717	24.301	1.00	23.08
	ATOM	1694	CB	SER	518	30.976	8.027	23.173	1.00	22.02
60	ATOM	1695	OG	SER	518	31.283	7.336	21.978	1.00	24.01
	ATOM	1696	C	SER	518	33.432	7.862	23.810	1.00	25.15

5	ATOM	1697	O	SER	518	34.111	6.866	23.532	1.00	22.94
	ATOM	1698	N	ASN	519	33.923	9.097	23.713	1.00	22.42
	ATOM	1699	CA	ASN	519	35.295	9.309	23.260	1.00	21.87
	ATOM	1700	CB	ASN	519	35.605	10.807	23.157	1.00	24.46
	ATOM	1701	CG	ASN	519	34.864	11.469	22.021	1.00	29.02
10	ATOM	1702	OD1	ASN	519	34.661	10.864	20.965	1.00	31.93
	ATOM	1703	ND2	ASN	519	34.459	12.715	22.224	1.00	28.81
	ATOM	1704	C	ASN	519	36.292	8.643	24.201	1.00	21.46
	ATOM	1705	O	ASN	519	37.251	8.015	23.752	1.00	23.56
	ATOM	1706	N	LYS	520	36.070	8.782	25.504	1.00	23.23
15	ATOM	1707	CA	LYS	520	36.964	8.171	26.488	1.00	26.35
	ATOM	1708	CB	LYS	520	36.581	8.592	27.912	1.00	27.53
	ATOM	1709	CG	LYS	520	36.618	10.101	28.174	1.00	33.74
	ATOM	1710	CD	LYS	520	37.962	10.710	27.811	1.00	42.09
	ATOM	1711	CE	LYS	520	39.047	10.307	28.802	1.00	43.97
20	ATOM	1712	NZ	LYS	520	39.858	11.480	29.254	1.00	48.07
	ATOM	1713	C	LYS	520	36.899	6.644	26.376	1.00	27.71
	ATOM	1714	O	LYS	520	37.913	5.957	26.501	1.00	27.15
	ATOM	1715	N	GLY	521	35.704	6.117	26.141	1.00	25.02
	ATOM	1716	CA	GLY	521	35.562	4.676	26.003	1.00	26.67
25	ATOM	1717	C	GLY	521	36.254	4.168	24.753	1.00	27.06
	ATOM	1718	O	GLY	521	36.924	3.128	24.775	1.00	26.84
	ATOM	1719	N	AMET	522	36.101	4.893	23.650	0.50	25.87
	ATOM	1720	N	BMET	522	36.095	4.908	23.658	0.50	27.62
	ATOM	1721	CA	AMET	522	36.727	4.491	22.401	0.50	27.27
30	ATOM	1722	CA	BMET	522	36.703	4.551	22.384	0.50	30.14
	ATOM	1723	CB	AMET	522	36.267	5.396	21.260	0.50	26.50
	ATOM	1724	CB	BMET	522	36.252	5.525	21.288	0.50	32.46
	ATOM	1725	CG	AMET	522	34.827	5.162	20.866	0.50	25.05
	ATOM	1726	CG	BMET	522	35.681	4.854	20.045	0.50	35.70
35	ATOM	1727	SD	AMET	522	34.585	3.587	20.020	0.50	27.07
	ATOM	1728	SD	BMET	522	34.197	5.672	19.408	0.50	40.01
	ATOM	1729	CE	AMET	522	33.142	4.017	19.031	0.50	31.29
	ATOM	1730	CE	BMET	522	34.733	6.085	17.745	0.50	42.12
	ATOM	1731	C	AMET	522	38.242	4.532	22.512	0.50	28.99
40	ATOM	1732	C	BMET	522	38.224	4.567	22.483	0.50	30.76
	ATOM	1733	O	AMET	522	38.939	3.743	21.870	0.50	31.65
	ATOM	1734	O	BMET	522	38.905	3.793	21.807	0.50	32.87
	ATOM	1735	N	GLU	523	38.749	5.452	23.324	1.00	30.85
	ATOM	1736	CA	GLU	523	40.190	5.576	23.513	1.00	34.09
45	ATOM	1737	CB	GLU	523	40.515	6.725	24.480	1.00	35.59
	ATOM	1738	CG	GLU	523	40.658	8.079	23.784	1.00	43.35
	ATOM	1739	CD	GLU	523	40.560	9.265	24.739	1.00	46.63
	ATOM	1740	OE1	GLU	523	39.832	10.240	24.416	1.00	47.64
	ATOM	1741	OE2	GLU	523	41.212	9.225	25.805	1.00	43.09
50	ATOM	1742	C	GLU	523	40.718	4.260	24.061	1.00	34.62
	ATOM	1743	O	GLU	523	41.733	3.747	23.596	1.00	33.87
	ATOM	1744	N	HIS	524	40.021	3.700	25.042	1.00	36.33
	ATOM	1745	CA	HIS	524	40.455	2.427	25.607	1.00	39.20
	ATOM	1746	CB	HIS	524	39.678	2.093	26.878	1.00	40.75
55	ATOM	1747	CG	HIS	524	40.061	0.774	27.473	1.00	48.10
	ATOM	1748	CD2	HIS	524	41.192	0.376	28.104	1.00	48.56
	ATOM	1749	ND1	HIS	524	39.247	-0.338	27.412	1.00	48.84
	ATOM	1750	CE1	HIS	524	39.859	-1.362	27.978	1.00	50.19
	ATOM	1751	NE2	HIS	524	41.041	-0.956	28.407	1.00	51.61
60	ATOM	1752	C	HIS	524	40.290	1.282	24.613	1.00	38.06
	ATOM	1753	O	HIS	524	41.226	0.521	24.371	1.00	38.18



5	ATOM	1754	N	LEU	525	39.101	1.162	24.034	1.00	36.96
	ATOM	1755	CA	LEU	525	38.831	0.093	23.084	1.00	37.40
	ATOM	1756	CB	LEU	525	37.416	0.241	22.514	1.00	35.89
	ATOM	1757	CG	LEU	525	36.268	0.107	23.527	1.00	33.17
	ATOM	1758	CD1	LEU	525	34.936	0.246	22.811	1.00	31.77
10	ATOM	1759	CD2	LEU	525	36.343	-1.240	24.238	1.00	35.92
	ATOM	1760	C	LEU	525	39.859	0.057	21.954	1.00	41.32
	ATOM	1761	O	LEU	525	40.244	-1.015	21.487	1.00	40.76
	ATOM	1762	N	TYR	526	40.314	1.227	21.522	1.00	43.68
	ATOM	1763	CA	TYR	526	41.300	1.297	20.449	1.00	49.00
15	ATOM	1764	CB	TYR	526	41.376	2.722	19.890	1.00	51.86
	ATOM	1765	CG	TYR	526	42.305	2.878	18.704	1.00	57.70
	ATOM	1766	CD1	TYR	526	41.835	2.718	17.400	1.00	58.93
	ATOM	1767	CE1	TYR	526	42.681	2.875	16.305	1.00	61.21
	ATOM	1768	CD2	TYR	526	43.653	3.200	18.883	1.00	58.58
20	ATOM	1769	CE2	TYR	526	44.510	3.359	17.790	1.00	61.15
	ATOM	1770	CZ	TYR	526	44.016	3.194	16.505	1.00	61.09
	ATOM	1771	OH	TYR	526	44.851	3.343	15.417	1.00	63.79
	ATOM	1772	C	TYR	526	42.671	0.871	20.964	1.00	50.14
	ATOM	1773	O	TYR	526	43.471	0.303	20.223	1.00	50.73
25	ATOM	1774	N	SER	527	42.930	1.139	22.240	1.00	52.72
	ATOM	1775	CA	SER	527	44.205	0.790	22.857	1.00	55.88
	ATOM	1776	CB	SER	527	44.351	1.516	24.199	1.00	55.00
	ATOM	1777	OG	SER	527	43.752	0.788	25.257	1.00	52.46
	ATOM	1778	C	SER	527	44.365	-0.718	23.054	1.00	60.39
30	ATOM	1779	O	SER	527	45.398	-1.185	23.534	1.00	60.43
	ATOM	1780	N	MET	528	43.335	-1.472	22.678	1.00	63.86
	ATOM	1781	CA	MET	528	43.347	-2.929	22.788	1.00	67.95
	ATOM	1782	CB	MET	528	42.534	-3.381	24.008	1.00	67.85
	ATOM	1783	CG	MET	528	41.237	-2.606	24.222	1.00	70.10
35	ATOM	1784	SD	MET	528	39.895	-3.569	24.983	1.00	71.70
	ATOM	1785	CE	MET	528	39.231	-4.412	23.554	1.00	72.57
	ATOM	1786	C	MET	528	42.726	-3.502	21.513	1.00	70.33
	ATOM	1787	O	MET	528	42.170	-4.602	21.513	1.00	72.43
	ATOM	1788	N	LYS	529	42.834	-2.739	20.428	1.00	71.53
40	ATOM	1789	CA	LYS	529	42.274	-3.122	19.136	1.00	72.00
	ATOM	1790	CB	LYS	529	42.508	-2.004	18.119	1.00	71.30
	ATOM	1791	C	LYS	529	42.813	-4.439	18.587	1.00	72.47
	ATOM	1792	O	LYS	529	43.990	-4.762	18.751	1.00	70.37
	ATOM	1793	N	CYS	530	41.932	-5.191	17.930	1.00	74.48
45	ATOM	1794	CA	CYS	530	42.279	-6.474	17.325	1.00	76.67
	ATOM	1795	CB	CYS	530	41.004	-7.245	16.952	1.00	77.23
	ATOM	1796	SG	CYS	530	40.447	-8.491	18.146	1.00	79.38
	ATOM	1797	C	CYS	530	43.098	-6.220	16.065	1.00	78.08
	ATOM	1798	O	CYS	530	43.241	-5.076	15.623	1.00	78.81
50	ATOM	1799	N	LYS	531	43.637	-7.289	15.487	1.00	78.22
	ATOM	1800	CA	LYS	531	44.424	-7.187	14.267	1.00	78.15
	ATOM	1801	CB	LYS	531	45.600	-8.182	14.305	1.00	78.33
	ATOM	1802	C	LYS	531	43.508	-7.467	13.067	1.00	77.93
	ATOM	1803	O	LYS	531	42.549	-6.734	12.839	1.00	78.07
55	ATOM	1804	N	ASN	532	43.784	-8.539	12.328	1.00	77.80
	ATOM	1805	CA	ASN	532	42.984	-8.902	11.152	1.00	77.30
	ATOM	1806	CB	ASN	532	43.550	-10.166	10.521	1.00	77.55
	ATOM	1807	C	ASN	532	41.485	-9.082	11.423	1.00	77.34
	ATOM	1808	O	ASN	532	40.904	-10.123	11.118	1.00	78.13
60	ATOM	1809	N	VAL	533	40.859	-8.055	11.988	1.00	76.13
	ATOM	1810	CA	VAL	533	39.436	-8.098	12.280	1.00	73.77

5	ATOM	1811	CB	VAL	533	39.155	-7.715	13.752	1.00	73.62
	ATOM	1812	CG1	VAL	533	39.690	-6.327	14.047	1.00	73.13
	ATOM	1813	CG2	VAL	533	37.662	-7.782	14.021	1.00	73.14
	ATOM	1814	C	VAL	533	38.685	-7.143	11.352	1.00	72.97
	ATOM	1815	O	VAL	533	39.024	-5.960	11.252	1.00	73.91
10	ATOM	1816	N	VAL	534	37.671	-7.666	10.666	1.00	70.02
	ATOM	1817	CA	VAL	534	36.866	-6.867	9.747	1.00	66.70
	ATOM	1818	CB	VAL	534	35.619	-7.646	9.328	1.00	67.32
	ATOM	1819	C	VAL	534	36.463	-5.541	10.393	1.00	63.87
	ATOM	1820	O	VAL	534	35.895	-5.519	11.486	1.00	63.55
15	ATOM	1821	N	PRO	535	36.756	-4.415	9.719	1.00	60.92
	ATOM	1822	CD	PRO	535	37.424	-4.354	8.408	1.00	61.01
	ATOM	1823	CA	PRO	535	36.424	-3.077	10.229	1.00	56.83
	ATOM	1824	CB	PRO	535	36.867	-2.135	9.107	1.00	58.70
	ATOM	1825	CG	PRO	535	37.023	-3.009	7.893	1.00	61.55
20	ATOM	1826	C	PRO	535	34.944	-2.902	10.571	1.00	52.90
	ATOM	1827	O	PRO	535	34.067	-3.461	9.908	1.00	52.01
	ATOM	1828	N	LEU	536	34.672	-2.120	11.610	1.00	48.60
	ATOM	1829	CA	LEU	536	33.301	-1.874	12.042	1.00	45.08
	ATOM	1830	CB	LEU	536	33.280	-0.796	13.128	1.00	44.35
25	ATOM	1831	CG	LEU	536	32.267	-0.911	14.273	1.00	43.48
	ATOM	1832	CD1	LEU	536	31.919	0.490	14.745	1.00	43.41
	ATOM	1833	CD2	LEU	536	31.022	-1.654	13.835	1.00	39.55
	ATOM	1834	C	LEU	536	32.434	-1.433	10.871	1.00	43.58
	ATOM	1835	O	LEU	536	31.287	-1.862	10.734	1.00	42.14
30	ATOM	1836	N	TYR	537	32.992	-0.575	10.024	1.00	43.02
	ATOM	1837	CA	TYR	537	32.269	-0.066	8.866	1.00	43.34
	ATOM	1838	CB	TYR	537	33.200	0.786	7.997	1.00	44.76
	ATOM	1839	CG	TYR	537	32.483	1.558	6.913	1.00	48.28
	ATOM	1840	CD1	TYR	537	32.190	0.964	5.687	1.00	48.46
35	ATOM	1841	CE1	TYR	537	31.504	1.660	4.693	1.00	52.48
	ATOM	1842	CD2	TYR	537	32.073	2.875	7.123	1.00	49.99
	ATOM	1843	CE2	TYR	537	31.383	3.584	6.135	1.00	53.73
	ATOM	1844	CZ	TYR	537	31.100	2.967	4.924	1.00	54.01
	ATOM	1845	OH	TYR	537	30.401	3.648	3.952	1.00	55.90
40	ATOM	1846	C	TYR	537	31.683	-1.199	8.032	1.00	43.15
	ATOM	1847	O	TYR	537	30.500	-1.191	7.696	1.00	41.54
	ATOM	1848	N	ASP	538	32.521	-2.175	7.702	1.00	44.67
	ATOM	1849	CA	ASP	538	32.097	-3.309	6.893	1.00	45.49
	ATOM	1850	CB	ASP	538	33.322	-4.126	6.479	1.00	51.32
45	ATOM	1851	CG	ASP	538	34.361	-3.284	5.748	1.00	56.17
	ATOM	1852	OD1	ASP	538	35.436	-3.820	5.396	1.00	57.29
	ATOM	1853	OD2	ASP	538	34.097	-2.079	5.526	1.00	59.24
	ATOM	1854	C	ASP	538	31.071	-4.195	7.587	1.00	43.48
	ATOM	1855	O	ASP	538	30.177	-4.738	6.940	1.00	43.95
50	ATOM	1856	N	LEU	539	31.193	-4.345	8.901	1.00	41.57
	ATOM	1857	CA	LEU	539	30.244	-5.157	9.654	1.00	39.11
	ATOM	1858	CB	LEU	539	30.734	-5.351	11.092	1.00	41.88
	ATOM	1859	CG	LEU	539	29.770	-6.065	12.044	1.00	46.11
	ATOM	1860	CD1	LEU	539	29.298	-7.379	11.423	1.00	46.99
55	ATOM	1861	CD2	LEU	539	30.474	-6.319	13.377	1.00	45.76
	ATOM	1862	C	LEU	539	28.891	-4.451	9.651	1.00	36.38
	ATOM	1863	O	LEU	539	27.849	-5.070	9.436	1.00	35.74
	ATOM	1864	N	LEU	540	28.919	-3.146	9.894	1.00	35.50
	ATOM	1865	CA	LEU	540	27.703	-2.336	9.903	1.00	35.59
60	ATOM	1866	CB	LEU	540	28.061	-0.877	10.219	1.00	37.63
	ATOM	1867	CG	LEU	540	27.856	-0.252	11.605	1.00	40.28

5	ATOM	1868	CD1	LEU	540	27.526	-1.299	12.645	1.00	38.55
	ATOM	1869	CD2	LEU	540	29.114	0.506	11.985	1.00	41.04
	ATOM	1870	C	LEU	540	27.060	-2.415	8.510	1.00	35.50
	ATOM	1871	O	LEU	540	25.846	-2.585	8.371	1.00	33.21
	ATOM	1872	N	LEU	541	27.892	-2.289	7.483	1.00	37.01
10	ATOM	1873	CA	LEU	541	27.418	-2.340	6.101	1.00	38.51
	ATOM	1874	CB	LEU	541	28.591	-2.152	5.145	1.00	39.67
	ATOM	1875	CG	LEU	541	28.301	-2.112	3.643	1.00	40.92
	ATOM	1876	CD1	LEU	541	27.184	-1.130	3.348	1.00	42.44
	ATOM	1877	CD2	LEU	541	29.572	-1.716	2.908	1.00	44.18
15	ATOM	1878	C	LEU	541	26.723	-3.676	5.833	1.00	39.75
	ATOM	1879	O	LEU	541	25.616	-3.713	5.297	1.00	36.48
	ATOM	1880	N	GLU	542	27.366	-4.770	6.230	1.00	40.88
	ATOM	1881	CA	GLU	542	26.790	-6.097	6.037	1.00	41.89
	ATOM	1882	CB	GLU	542	27.719	-7.170	6.620	1.00	44.11
20	ATOM	1883	CG	GLU	542	27.010	-8.457	7.052	1.00	50.60
	ATOM	1884	CD	GLU	542	26.434	-9.245	5.887	1.00	55.80
	ATOM	1885	OE1	GLU	542	25.570	-10.117	6.130	1.00	58.81
	ATOM	1886	OE2	GLU	542	26.842	-8.996	4.728	1.00	57.19
	ATOM	1887	C	GLU	542	25.414	-6.195	6.691	1.00	41.58
25	ATOM	1888	O	GLU	542	24.472	-6.720	6.102	1.00	42.82
	ATOM	1889	N	MET	543	25.298	-5.686	7.915	1.00	40.09
	ATOM	1890	CA	MET	543	24.036	-5.731	8.634	1.00	36.43
	ATOM	1891	CB	MET	543	24.270	-5.424	10.111	1.00	39.95
	ATOM	1892	CG	MET	543	25.137	-6.459	10.808	1.00	41.95
30	ATOM	1893	SD	MET	543	24.918	-6.445	12.604	1.00	47.17
	ATOM	1894	CE	MET	543	25.324	-4.749	12.964	1.00	40.88
	ATOM	1895	C	MET	543	23.001	-4.769	8.072	1.00	35.02
	ATOM	1896	O	MET	543	21.808	-5.073	8.048	1.00	35.31
	ATOM	1897	N	LEU	544	23.457	-3.605	7.629	1.00	32.90
35	ATOM	1898	CA	LEU	544	22.559	-2.603	7.074	1.00	36.88
	ATOM	1899	CB	LEU	544	23.225	-1.226	7.111	1.00	34.51
	ATOM	1900	CG	LEU	544	23.268	-0.562	8.490	1.00	31.94
	ATOM	1901	CD1	LEU	544	24.284	0.564	8.478	1.00	32.27
	ATOM	1902	CD2	LEU	544	21.897	-0.029	8.846	1.00	29.02
40	ATOM	1903	C	LEU	544	22.148	-2.941	5.640	1.00	38.94
	ATOM	1904	O	LEU	544	20.971	-2.842	5.294	1.00	39.52
	ATOM	1905	N	ASP	545	23.118	-3.338	4.817	1.00	41.05
	ATOM	1906	CA	ASP	545	22.850	-3.685	3.418	1.00	40.78
	ATOM	1907	CB	ASP	545	24.159	-3.780	2.620	1.00	37.75
45	ATOM	1908	CG	ASP	545	23.922	-3.937	1.120	1.00	35.19
	ATOM	1909	OD1	ASP	545	24.881	-4.265	0.380	1.00	33.48
	ATOM	1910	OD2	ASP	545	22.768	-3.734	0.691	1.00	31.33
	ATOM	1911	C	ASP	545	22.116	-5.015	3.349	1.00	42.87
	ATOM	1912	O	ASP	545	22.681	-6.030	2.929	1.00	44.32
50	ATOM	1913	N	ALA	546	20.853	-5.009	3.755	1.00	43.49
	ATOM	1914	CA	ALA	546	20.069	-6.229	3.746	1.00	46.96
	ATOM	1915	CB	ALA	546	19.213	-6.305	5.006	1.00	47.82
	ATOM	1916	C	ALA	546	19.193	-6.362	2.508	1.00	49.55
	ATOM	1917	O	ALA	546	18.804	-5.368	1.883	1.00	48.75
55	ATOM	1918	N	HIS	547	18.895	-7.606	2.152	1.00	50.98
	ATOM	1919	CA	HIS	547	18.042	-7.884	1.006	1.00	53.77
	ATOM	1920	CB	HIS	547	18.431	-9.223	0.369	1.00	52.69
	ATOM	1921	CG	HIS	547	18.395	-10.382	1.317	1.00	55.05
	ATOM	1922	CD2	HIS	547	17.477	-10.752	2.242	1.00	53.94
60	ATOM	1923	ND1	HIS	547	19.395	-11.329	1.371	1.00	56.23
	ATOM	1924	CE1	HIS	547	19.095	-12.232	2.286	1.00	55.36

5	ATOM	1925	NE2	HIS	547	17.936	-11.906	2.830	1.00	57.01
	ATOM	1926	C	HIS	547	16.603	-7.936	1.518	1.00	55.69
	ATOM	1927	O	HIS	547	16.362	-7.796	2.720	1.00	54.30
	ATOM	1928	N	ARG	548	15.653	-8.139	0.612	1.00	57.00
	ATOM	1929	CA	ARG	548	14.245	-8.212	0.987	1.00	60.65
10	ATOM	1930	CB	ARG	548	13.432	-7.171	0.208	1.00	62.69
	ATOM	1931	CG	ARG	548	14.272	-6.222	-0.637	1.00	67.54
	ATOM	1932	CD	ARG	548	13.448	-5.061	-1.171	1.00	71.92
	ATOM	1933	NE	ARG	548	13.702	-3.826	-0.432	1.00	76.95
	ATOM	1934	CZ	ARG	548	14.864	-3.178	-0.429	1.00	79.04
15	ATOM	1935	NH1	ARG	548	15.891	-3.644	-1.128	1.00	80.66
	ATOM	1936	NH2	ARG	548	15.001	-2.063	0.278	1.00	80.39
	ATOM	1937	C	ARG	548	13.695	-9.608	0.711	1.00	61.65
	ATOM	1938	O	ARG	548	12.500	-9.781	0.466	1.00	62.05
	ATOM	1939	N	LEU	549	14.576	-10.603	0.756	1.00	62.39
20	ATOM	1940	CA	LEU	549	14.188	-11.985	0.507	1.00	64.02
	ATOM	1941	CB	LEU	549	15.433	-12.828	0.195	1.00	62.14
	ATOM	1942	CG	LEU	549	16.461	-12.191	-0.753	1.00	60.76
	ATOM	1943	CD1	LEU	549	17.699	-13.074	-0.878	1.00	57.77
	ATOM	1944	CD2	LEU	549	15.823	-11.972	-2.108	1.00	58.38
25	ATOM	1945	C	LEU	549	13.431	-12.574	1.702	1.00	66.65
	ATOM	1946	O	LEU	549	12.759	-13.600	1.577	1.00	67.15
	ATOM	1947	N	HIS	550	13.541	-11.920	2.856	1.00	67.72
	ATOM	1948	CA	HIS	550	12.858	-12.378	4.065	1.00	69.93
	ATOM	1949	CB	HIS	550	13.753	-12.190	5.298	1.00	70.76
30	ATOM	1950	CG	HIS	550	14.977	-13.054	5.306	1.00	71.50
	ATOM	1951	CD2	HIS	550	15.539	-13.821	4.341	1.00	71.63
	ATOM	1952	ND1	HIS	550	15.793	-13.172	6.411	1.00	71.98
	ATOM	1953	CE1	HIS	550	16.805	-13.972	6.126	1.00	72.04
	ATOM	1954	NE2	HIS	550	16.674	-14.379	4.876	1.00	71.39
35	ATOM	1955	C	HIS	550	11.556	-11.603	4.275	1.00	71.15
	ATOM	1956	O	HIS	550	10.940	-11.684	5.340	1.00	70.66
	ATOM	1957	N	ALA	551	11.143	-10.851	3.258	1.00	72.22
	ATOM	1958	CA	ALA	551	9.919	-10.057	3.338	1.00	73.58
	ATOM	1959	CB	ALA	551	9.904	-9.014	2.221	1.00	73.21
40	ATOM	1960	C	ALA	551	8.658	-10.920	3.266	1.00	74.69
	ATOM	1961	O	ALA	551	7.684	-10.474	2.621	1.00	76.12
	ATOM	1962	OXT	ALA	551	8.651	-12.025	3.852	1.00	73.79
	HETATM	1963	C10	OHT	600	30.581	1.481	29.471	1.00	26.84
	HETATM	1964	C9	OHT	600	30.713	-0.043	29.358	1.00	22.85
45	HETATM	1965	C8	OHT	600	31.366	-0.385	28.037	1.00	25.56
	HETATM	1966	C11	OHT	600	32.761	0.051	27.916	1.00	27.51
	HETATM	1967	C16	OHT	600	33.218	0.797	26.797	1.00	28.35
	HETATM	1968	C15	OHT	600	34.551	1.237	26.747	1.00	30.39
	HETATM	1969	C14	OHT	600	35.443	0.923	27.792	1.00	30.23
50	HETATM	1970	C13	OHT	600	35.004	0.185	28.890	1.00	31.45
	HETATM	1971	C12	OHT	600	33.666	-0.241	28.955	1.00	27.93
	HETATM	1972	C7	OHT	600	30.682	-1.089	27.077	1.00	24.41
	HETATM	1973	C1	OHT	600	29.211	-1.258	27.052	1.00	24.26
	HETATM	1974	C2	OHT	600	28.644	-2.526	26.706	1.00	25.92
55	HETATM	1975	C3	OHT	600	27.254	-2.668	26.580	1.00	26.32
	HETATM	1976	C4	OHT	600	26.438	-1.553	26.813	1.00	29.02
	HETATM	1977	O4	OHT	600	25.072	-1.605	26.716	1.00	28.42
	HETATM	1978	C5	OHT	600	26.980	-0.286	27.130	1.00	26.98
	HETATM	1979	C6	OHT	600	28.362	-0.147	27.231	1.00	25.23
60	HETATM	1980	C17	OHT	600	31.370	-1.692	25.942	1.00	26.61
	HETATM	1981	C18	OHT	600	32.508	-2.498	26.151	1.00	26.77

5	HETATM	1982	C19	OHT	600	33.166	-3.052	25.072	1.00	27.50
	HETATM	1983	C20	OHT	600	32.676	-2.794	23.786	1.00	27.50
	HETATM	1984	O20	OHT	600	33.206	-3.566	22.795	1.00	31.35
	HETATM	1985	C23	OHT	600	33.009	-3.135	21.448	1.00	40.09
	HETATM	1986	C24	OHT	600	34.226	-3.490	20.575	1.00	44.80
10	HETATM	1987	N24	OHT	600	34.141	-4.901	20.203	1.00	49.00
	HETATM	1988	C25	OHT	600	33.375	-5.040	18.933	1.00	51.64
	HETATM	1989	C26	OHT	600	35.495	-5.459	20.004	1.00	52.06
	HETATM	1990	C21	OHT	600	31.540	-2.005	23.558	1.00	27.19
	HETATM	1991	C22	OHT	600	30.892	-1.450	24.645	1.00	27.92
15	HETATM	1992	O1	HOH	1	20.714	-12.010	23.057	1.00	27.20
	HETATM	1993	O1	HOH	2	22.563	-0.070	25.819	1.00	25.77
	HETATM	1994	O1	HOH	3	25.183	19.202	23.149	1.00	42.52
	HETATM	1995	O1	HOH	4	35.158	5.823	37.390	1.00	33.92
	HETATM	1996	O1	HOH	5	22.116	-9.922	18.914	1.00	30.18
20	HETATM	1997	O1	HOH	6	29.812	6.536	19.652	1.00	26.11
	HETATM	1998	O1	HOH	7	13.362	4.463	20.376	1.00	29.40
	HETATM	1999	O1	HOH	8	19.799	-11.295	20.187	1.00	28.70
	HETATM	2000	O1	HOH	9	21.205	1.466	23.794	1.00	22.47
	HETATM	2001	O1	HOH	10	21.177	-4.961	29.066	1.00	33.00
25	HETATM	2002	O1	HOH	11	18.591	1.863	20.518	1.00	32.59
	HETATM	2003	O1	HOH	12	16.298	21.566	15.992	1.00	33.42
	HETATM	2004	O1	HOH	13	18.611	1.976	24.494	1.00	29.70
	HETATM	2005	O1	HOH	14	38.009	8.910	21.156	1.00	39.92
	HETATM	2006	O1	HOH	15	26.549	11.664	18.080	1.00	30.25
30	HETATM	2007	O1	HOH	16	20.282	-4.239	26.512	1.00	32.70
	HETATM	2008	O1	HOH	17	32.858	8.754	20.237	1.00	29.88
	HETATM	2009	O1	HOH	18	8.497	16.136	29.934	1.00	46.80
	HETATM	2010	O1	HOH	19	21.940	19.301	31.632	1.00	35.72
	HETATM	2011	O1	HOH	20	35.153	2.682	14.122	1.00	41.02
35	HETATM	2012	O1	HOH	21	20.358	-2.268	21.013	1.00	29.43
	HETATM	2013	O1	HOH	22	35.562	10.036	36.334	1.00	41.37
	HETATM	2014	O1	HOH	23	17.248	18.187	17.571	1.00	33.96
	HETATM	2015	O1	HOH	24	18.445	20.973	12.346	1.00	43.44
	HETATM	2016	O1	HOH	25	12.152	23.054	33.132	1.00	36.04
40	HETATM	2017	O1	HOH	26	13.181	22.222	9.699	1.00	37.03
	HETATM	2018	O1	HOH	27	19.399	-6.090	12.808	1.00	44.86
	HETATM	2019	O1	HOH	28	37.895	13.599	31.395	1.00	47.26
	HETATM	2020	O1	HOH	29	11.570	6.212	7.962	1.00	51.10
	HETATM	2021	O1	HOH	30	20.172	-2.568	23.445	1.00	51.70
45	HETATM	2022	O1	HOH	31	36.402	-5.369	23.729	1.00	58.20
	HETATM	2023	O1	HOH	32	25.127	13.802	19.187	1.00	35.29
	HETATM	2024	O1	HOH	33	23.181	4.937	38.538	1.00	33.77
	HETATM	2025	O1	HOH	34	20.550	0.421	21.276	1.00	29.12
	HETATM	2026	O1	HOH	35	39.599	13.954	27.312	1.00	44.08
50	HETATM	2027	O1	HOH	36	26.445	13.863	21.285	1.00	34.97
	HETATM	2028	O1	HOH	37	13.759	5.079	9.108	1.00	38.54
	HETATM	2029	O1	HOH	38	14.150	24.731	34.529	1.00	49.72
	HETATM	2030	O1	HOH	39	21.060	13.886	-6.319	1.00	59.79
	HETATM	2031	O1	HOH	40	32.215	6.217	8.726	1.00	60.22
55	HETATM	2032	O1	HOH	41	35.105	15.704	9.069	1.00	45.15
	HETATM	2033	O1	HOH	42	11.427	19.451	9.903	1.00	38.56
	HETATM	2034	O1	HOH	43	19.662	23.472	10.333	1.00	47.71
	HETATM	2035	O1	HOH	44	9.231	3.690	12.337	1.00	45.98
	HETATM	2036	O1	HOH	45	15.313	-6.036	17.192	1.00	39.07
60	HETATM	2037	O1	HOH	46	15.517	-3.266	17.907	1.00	37.67
	HETATM	2038	O1	HOH	47	28.784	-16.713	25.163	1.00	55.44

5	HETATM	2039	01	HOH	48	27.868	-10.898	28.271	1.00	31.27
	HETATM	2040	01	HOH	49	6.955	13.568	28.233	1.00	48.83
	HETATM	2041	01	HOH	50	22.051	-15.030	28.603	1.00	36.91
	HETATM	2042	01	HOH	51	7.026	31.002	30.284	1.00	46.73
	HETATM	2043	01	HOH	52	-1.489	12.385	15.164	1.00	51.17
10	HETATM	2044	01	HOH	53	3.499	6.444	14.452	1.00	50.38
	HETATM	2045	01	HOH	54	18.655	-2.048	25.518	1.00	52.29
	HETATM	2046	01	HOH	55	28.188	-15.195	38.996	1.00	55.22
	HETATM	2047	01	HOH	56	35.275	-10.556	38.061	1.00	57.39
	HETATM	2048	01	HOH	57	37.771	-9.103	34.605	1.00	54.17
15	HETATM	2049	01	HOH	58	31.403	-3.039	17.983	1.00	46.80
	HETATM	2050	01	HOH	59	30.455	-6.352	17.005	1.00	47.05
	HETATM	2051	01	HOH	60	25.985	8.255	0.416	1.00	43.32
	HETATM	2052	01	HOH	61	35.679	0.749	10.462	1.00	42.99
	HETATM	2053	01	HOH	62	14.741	4.029	33.936	1.00	49.59
20	HETATM	2054	01	HOH	63	16.333	2.592	35.952	1.00	45.13
	HETATM	2055	01	HOH	64	23.809	7.186	39.798	1.00	45.36
	HETATM	2056	01	HOH	65	27.012	-1.948	46.995	1.00	63.39
	HETATM	2057	01	HOH	66	25.956	-6.422	42.144	1.00	44.94
	HETATM	2058	01	HOH	67	23.510	-8.414	39.036	1.00	39.06
25	HETATM	2059	01	HOH	68	41.475	0.971	33.110	1.00	55.50
	HETATM	2060	01	HOH	69	36.519	8.863	38.836	1.00	41.56
	HETATM	2061	01	HOH	70	30.111	14.823	12.793	1.00	44.58
	HETATM	2062	01	HOH	71	26.850	-6.092	1.594	1.00	40.15
	HETATM	2063	01	HOH	72	20.448	-3.169	1.055	1.00	42.50
30	HETATM	2064	01	HOH	73	33.896	3.047	16.172	1.00	46.39
	HETATM	2065	01	HOH	74	16.884	0.446	26.043	1.00	61.50
	HETATM	2066	01	HOH	75	18.595	0.296	27.866	1.00	47.33
	HETATM	2067	01	HOH	76	6.166	21.439	19.124	1.00	47.94
	HETATM	2068	01	HOH	77	18.484	20.060	16.232	1.00	35.52
35	HETATM	2069	01	HOH	78	1.985	23.265	29.187	1.00	46.42
	HETATM	2070	01	HOH	79	12.729	30.461	27.530	1.00	62.79
END										

5 WHAT IS CLAIMED IS:

1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

10 modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof,

screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and

15 identifying a test compound that modulates coactivator binding to said nuclear receptor.

2. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.

20

3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

25

4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

30

5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and  
35 helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

8. The method of claim 1, wherein said nuclear receptor coactivator binding site  
10 comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.

9. The method of any one of claims 5 through 8, wherein said nuclear receptor is  
15 selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

10. The method of claim 1, wherein said screening is *in vitro*.

11. The method of claim 10, wherein said screening is high throughput screening.  
20

12. The method of claim 1, wherein said assay is a biological assay.

13. The method of claim 1, wherein said test compound is from a library of compounds.  
25

14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.

15. The method of claim 14, wherein said test compound is a small organic molecule, a  
30 peptide, or peptidomimetic.

16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.

17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear  
35 receptor, said method comprising the steps of:

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;



5 modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

10

18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising  
15 structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root  
20 mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

19. The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.

20. The machine readable storage medium of claim 19, wherein said thyroid receptor is human.

21. The machine readable storage medium of claim 20, wherein said molecule is peptide

22. The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.

23. The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a  
35 homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

5           24.    A machine-readable data storage medium comprising a data storage material  
encoded with a first set of machine readable data which, when combined with a second set of  
machine readable data, using a machine programmed with instructions for using said first set of data  
and said second set of data, can determine at least a portion of the structure coordinates  
corresponding to the second set of machine readable data, wherein: said first set of data comprises a  
10   Fourier transform of at least a portion of the structural coordinates selected from the group  
consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray  
diffraction pattern of a molecule or molecular complex.

          25.    A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator  
15   binding site of said nuclear receptor.

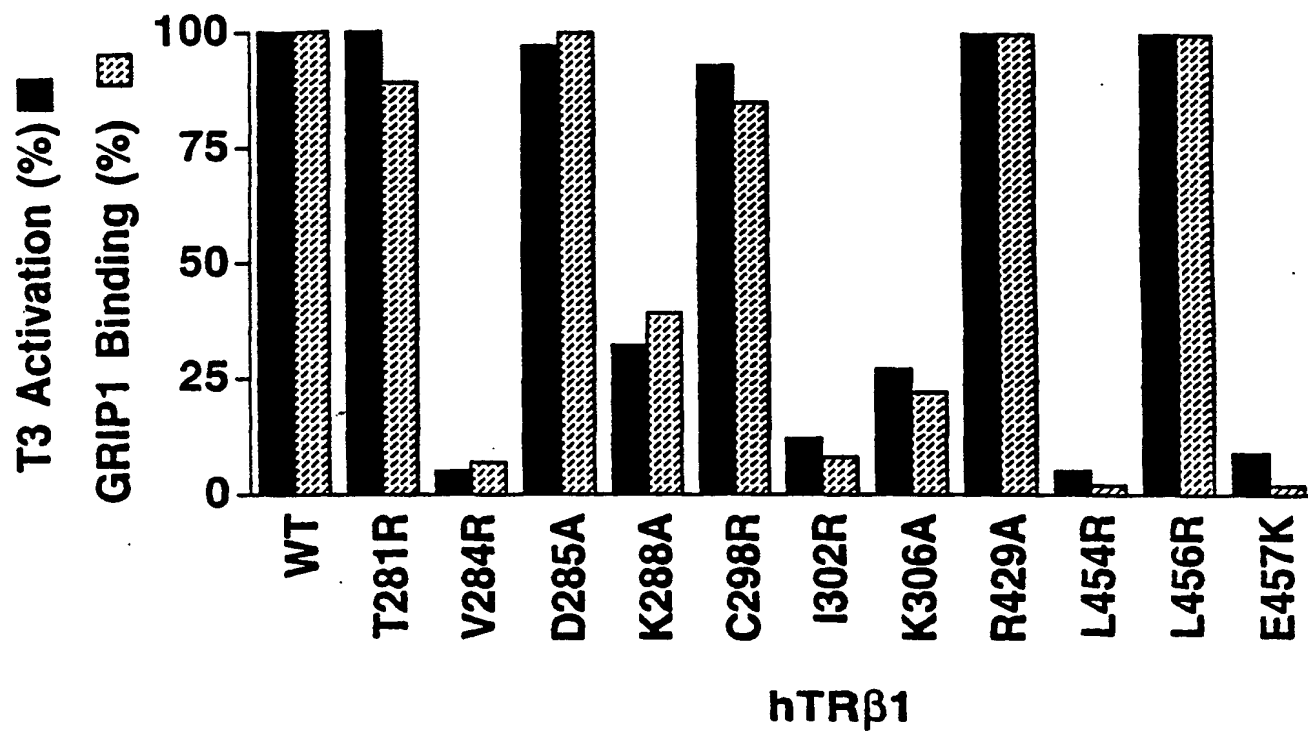
          26.    The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.

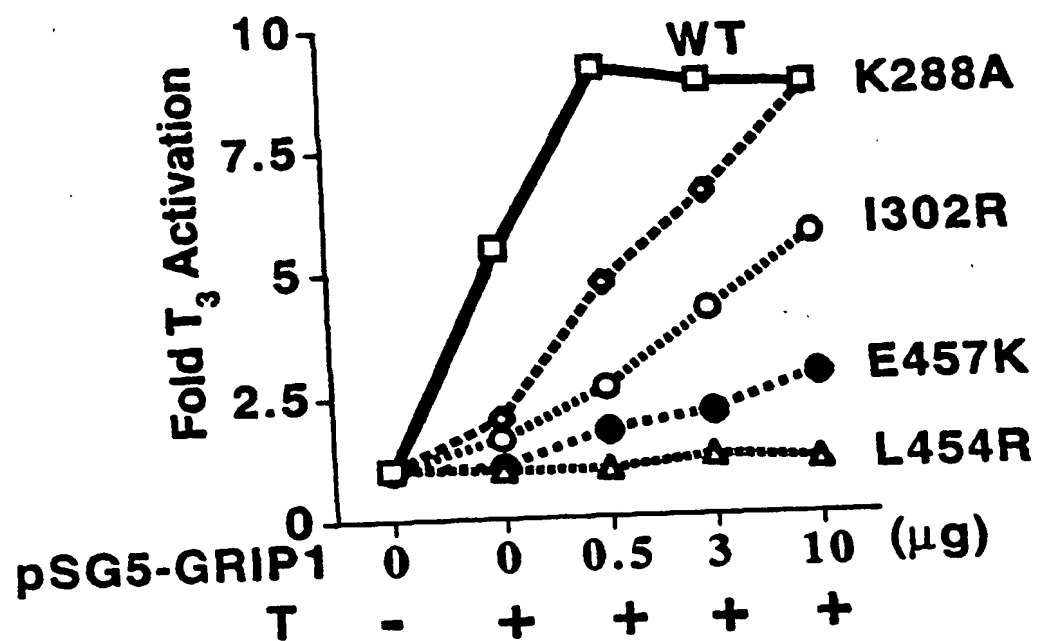
          27.    The cocrystal of claim 26, wherein said thyroid receptor is human.  
20

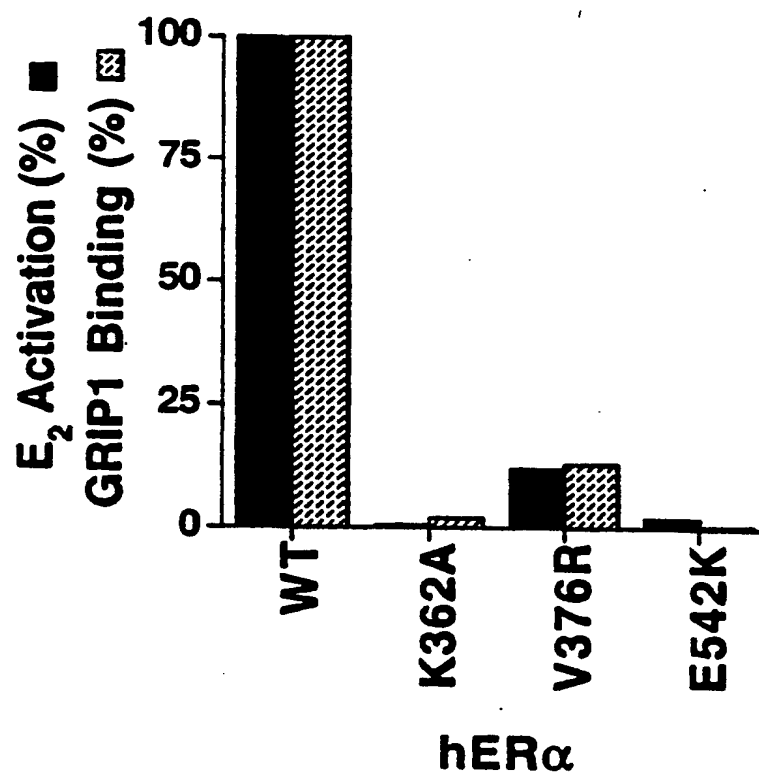
          28.    The cocrystal of claim 27, wherein said molecule is peptide.

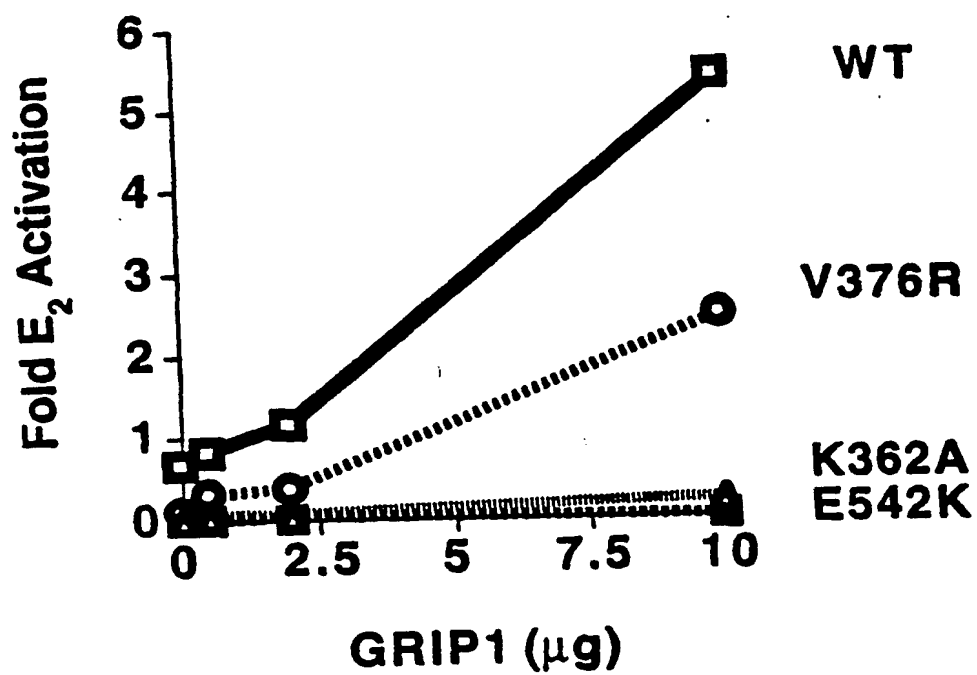
          29.    The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid  
sequence or derivative thereof.  
25

          30.    A compound identified according to the method of claim 1.

**FIGURE 1**

**FIGURE 2**

**FIGURE 3**

**FIGURE 4**

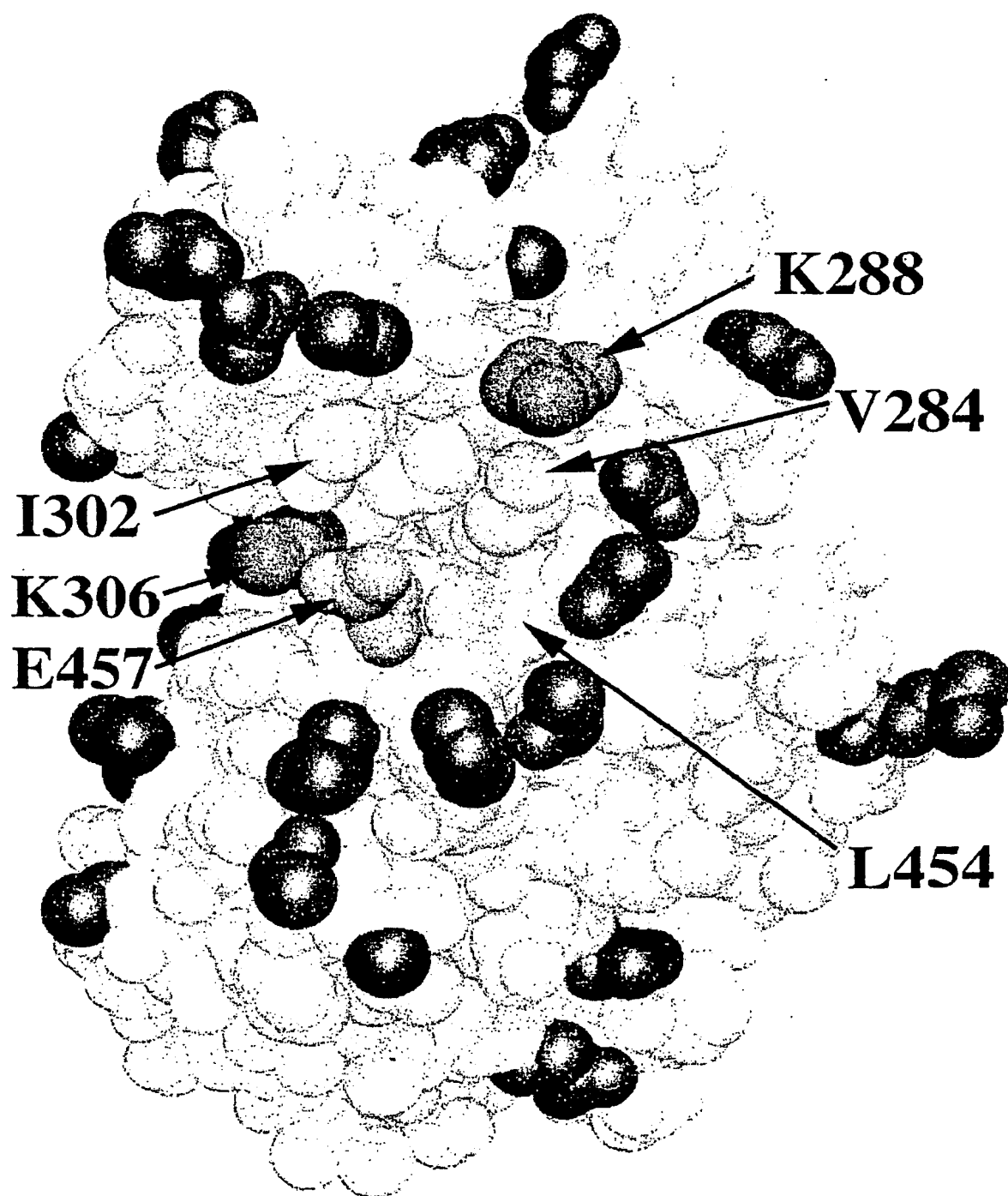


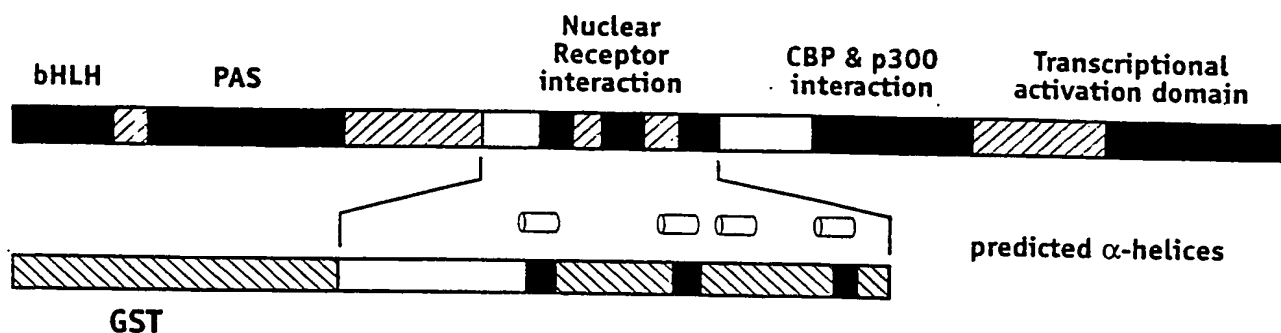
FIG. 5

# FIGURE 6

	bHLH	PAS	Nuclear Receptor interaction	CBP & p300 interaction	Transcriptional activation domain
			1	2	3
1			SEQ ID NO: 5 Grip1	AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS	
			SEQ ID NO: 8 Tif2	ADGQSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS	
			SEQ ID NO: 11 NcoA-2	AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLPS	
			SEQ ID NO: 14 RAC3	AENQRGPLESKGHKLLQLLTCSSDRGHSSLTN	
			SEQ ID NO: 17 AIB1, TRAM-1	AENQRGPLESKGHKLLQLLTCSSDRGHSSLTN	
			SEQ ID NO: 20 p/CIP	SETPRGPLESKGHKLLQLLTCSSDRGHSSLTN	
			SEQ ID NO: 23 SRC1	SEGDSKY--SQTSHKLVQLLTTTAEQQLRHADID	
			SEQ ID NO: 26 Consensus	.....S....KLhQLLT,....	
2			SEQ ID NO: 6 Grip1	PGSTHGTSLKEKHILHRLLDSSSPVDLAKLTA	
			SEQ ID NO: 9 Tif2	SGSTHGTSLKEKHILHRLLDSSSPVDLAKLTA	
			SEQ ID NO: 12 NcoA-2	PGSTHGTSLKEKHILHRLLDSSSPVDLAKLTA	
			SEQ ID NO: 15 RAC3	TSNMHGSLLOEKHRILHKLLQNGNSPAEVAKITA	
			SEQ ID NO: 18 AIB1, TRAM-1	TSNMHGSLLOEKHRILHKLLQNGNSPAEVAKITA	
			SEQ ID NO: 21 p/CIP	TSNVHGSLLOEKHRILHKLLQNGNSPAEVAKITA	
			SEQ ID NO: 24 SRC1	TCPSSHSSSLTERHKILHRLLOE.GSPSDITTLV	
			SEQ ID NO: 27 Consensus	.....L.E+H+ILH+LLQ...SP.-h..	
3			SEQ ID NO: 7 Grip1	EPASPKKKE---NALLRYLLDKDDTKDIGLPEIT	
			SEQ ID NO: 10 Tif2	EPVSPKKKE---NALLRYLLDKDDTKDIGLPEIT	
			SEQ ID NO: 13 NcoA-2	EPASPKKKE---NALLRYLLDKDDTKDIGLPSIT	
			SEQ ID NO: 16 RAC3	EQLSPKKKE--NNALLRYLLDRDDPSDVLAKKLQ	
			SEQ ID NO: 19 AIB1, TRAM-1	EQLSPKKKE--NNALLRYLLDRDDPSDALSKELO	
			SEQ ID NO: 22 p/CIP	EQLSPKKKE--NNALLRYLLDRDDPSDALSKELO	
			SEQ ID NO: 25 SRC1	ELDAAKKESKDHQLLRLLDKDEKDLRSTPNLC	
			SEQ ID NO: 28 Consensus	E....KKKE....LLRYLLD+D-.....h.	
			Overall Consensus (SEQ ID NO: 1)	.....LXXLL.....	

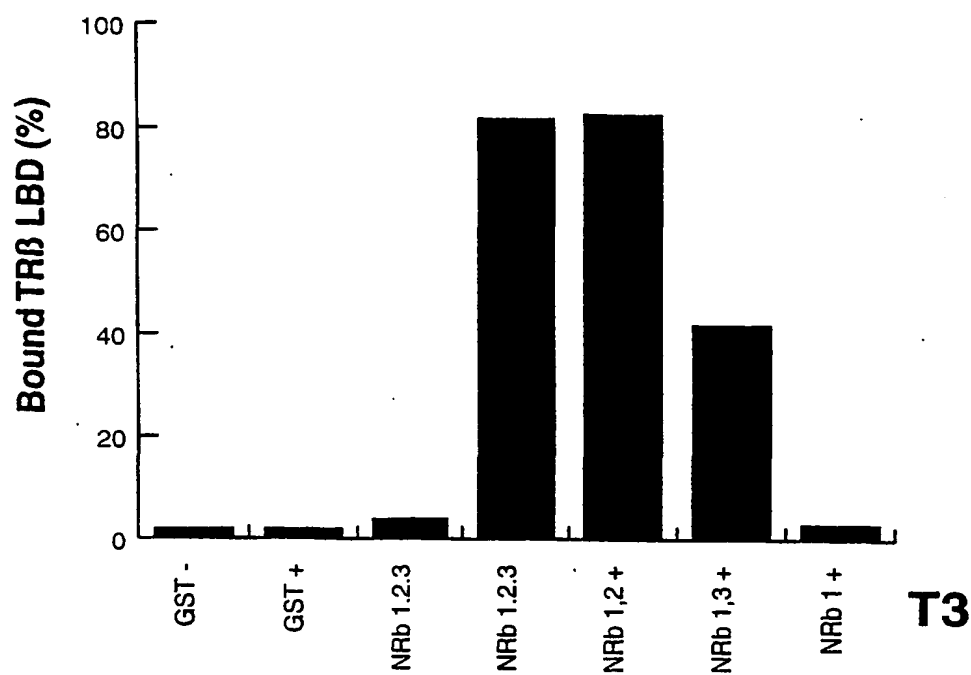


# FIGURE 7a

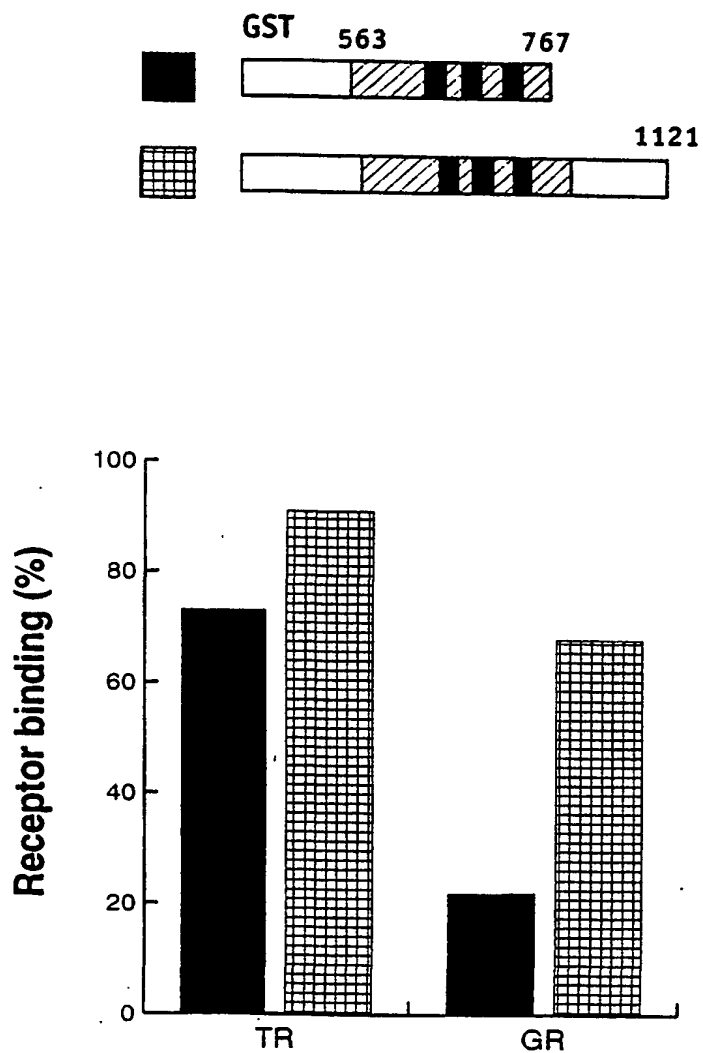


	NR-box1 residues 15-21 SEQ ID NO: 5	NR-box1 residues 15-21 SEQ ID NO: 6	NR box3 residues 15-21 SEQ ID NO: 7
NRb 1,2,3	KLLQLLT . . . . .	ILHRLLQ . . . . .	LLRYLLD
NRb 1,2	KLLQLLT . . . . .	ILHRLLQ . . . . .	AARAAAD
NRb 1,3	KLLQLLT . . . . .	AAHRAAQ . . . . .	LLRYLLD
NRb 1	KLLQLLT . . . . .	AAHRAAQ . . . . .	AARAAAD

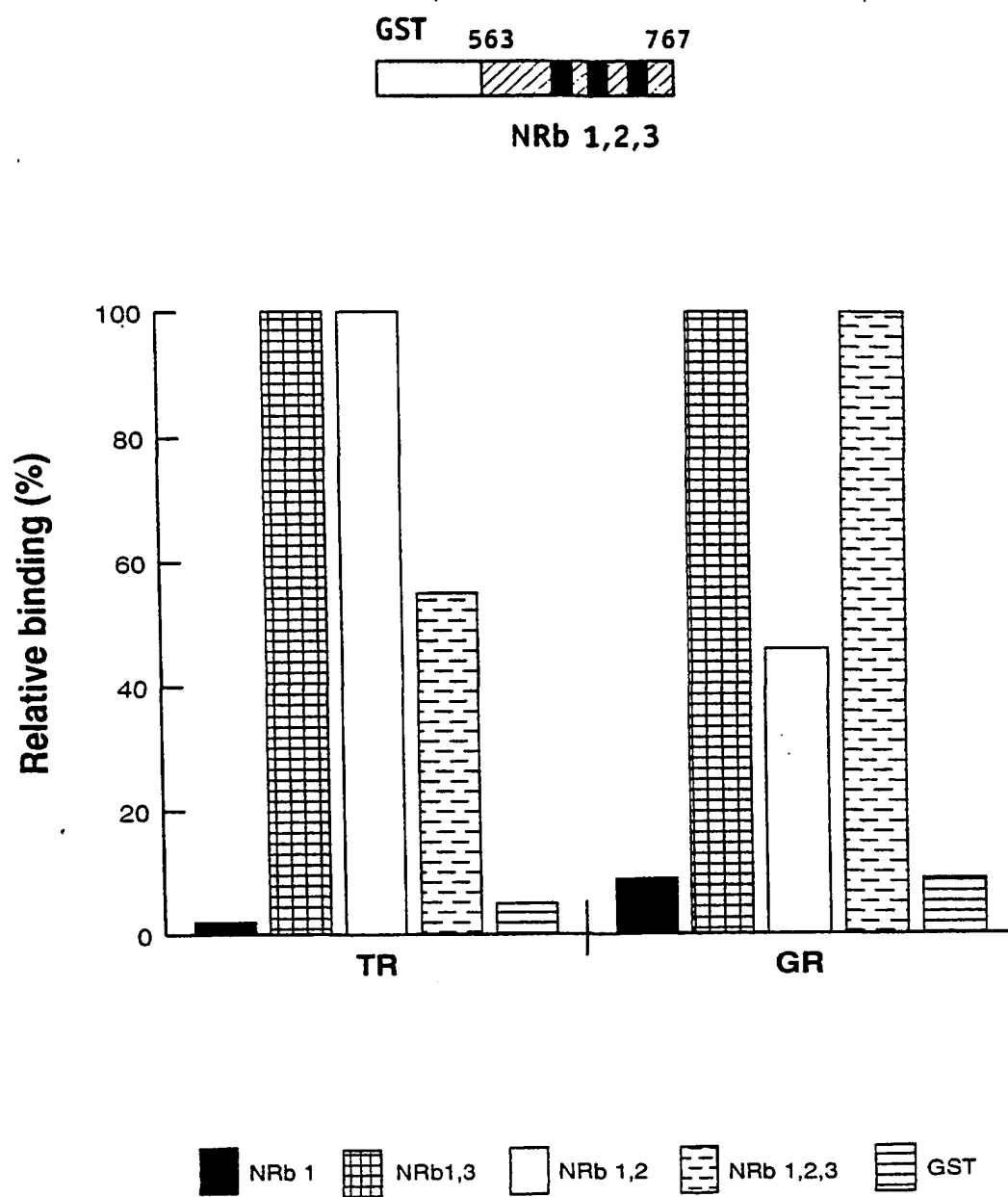
# FIGURE 7b



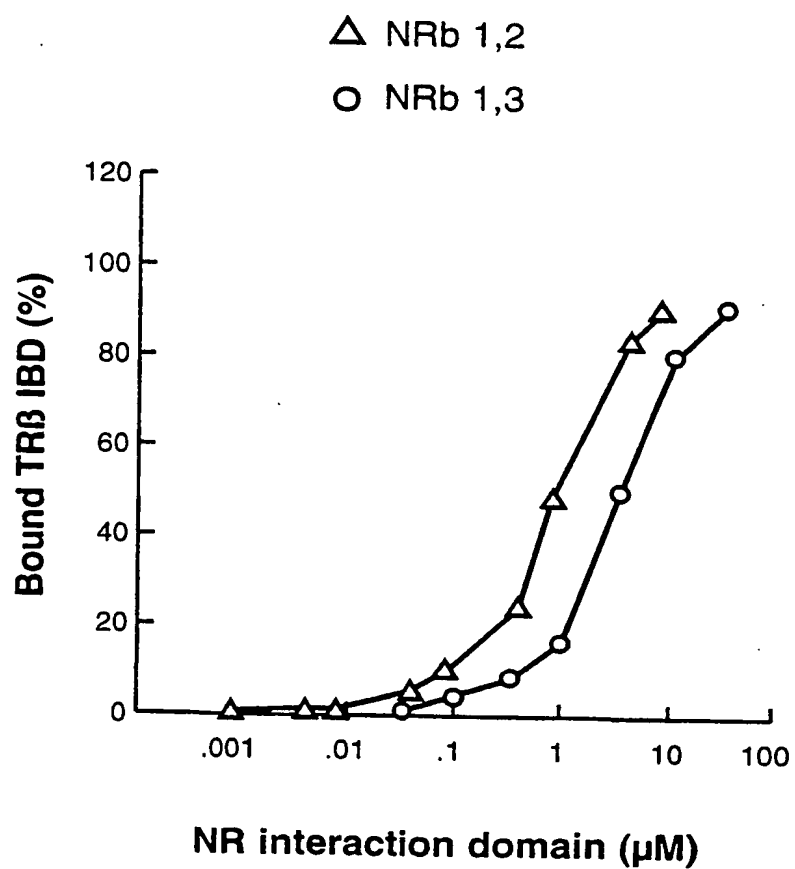
## FIGURE 8a



## FIGURE 8b

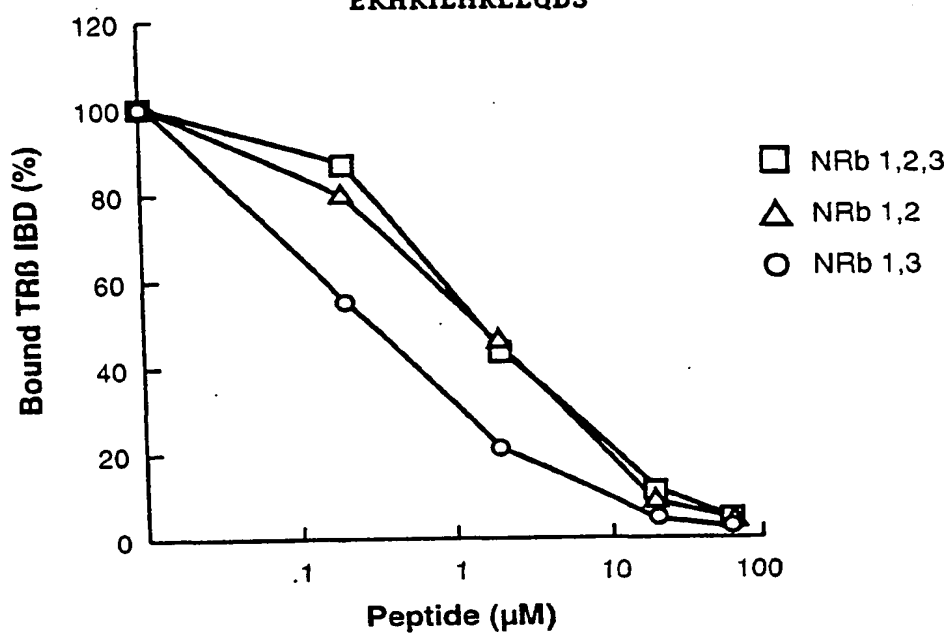


# FIGURE 9a

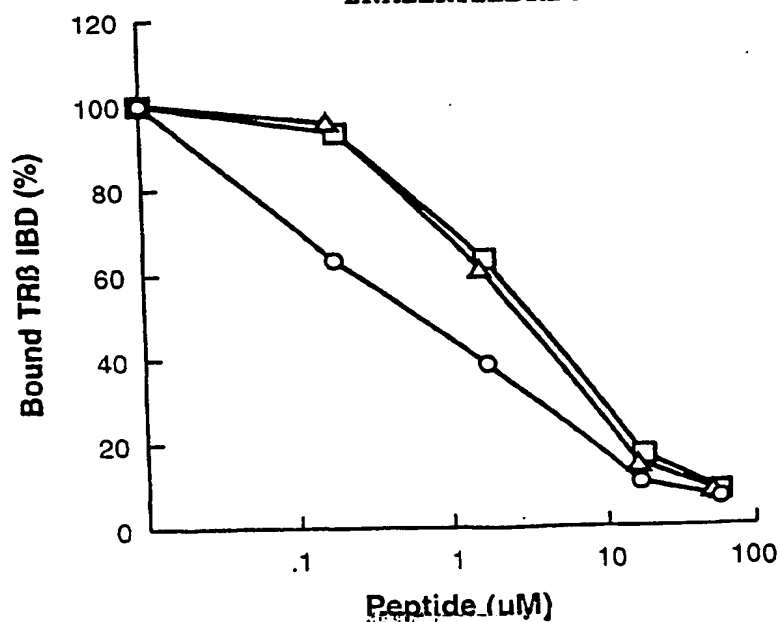


**FIGURE 9b**

NR-box 2 peptide  
EKHKILHRLIQDS



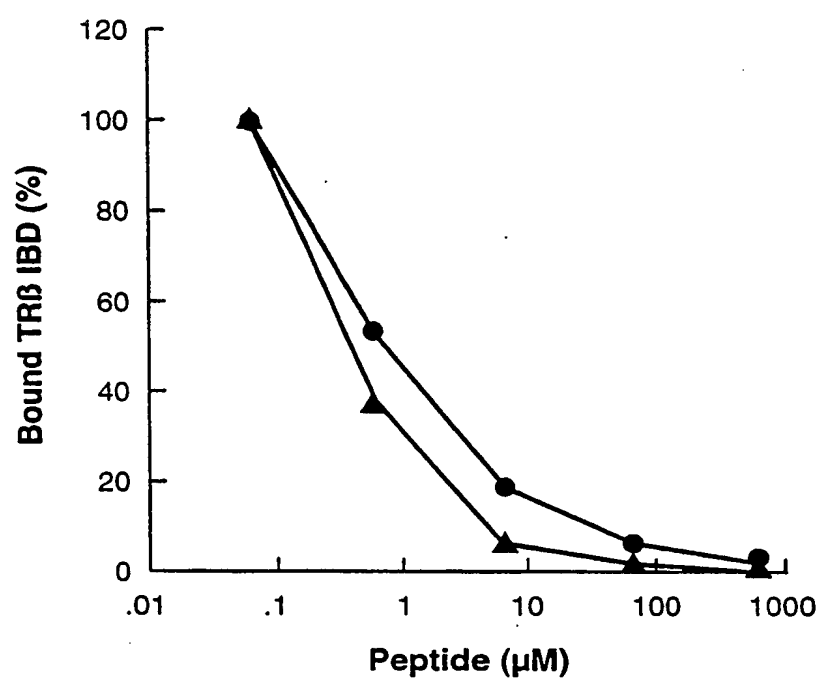
NR-box 3 peptide  
ENALLRYLLDKDO



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# FIGURE 10a

NR-box 2



● residues 11-23

EKHK

ILHRL

QDS

▲ residues 7-24

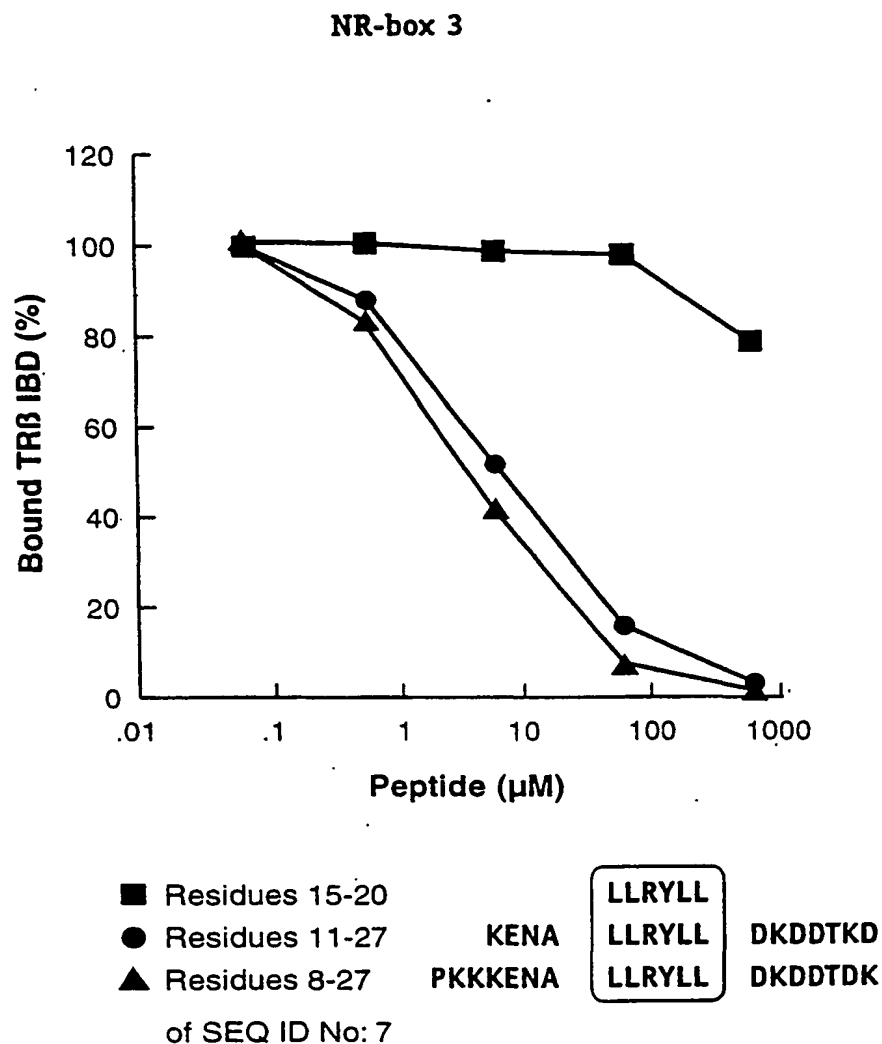
TSLKEKHK

ILHRL

QDSS

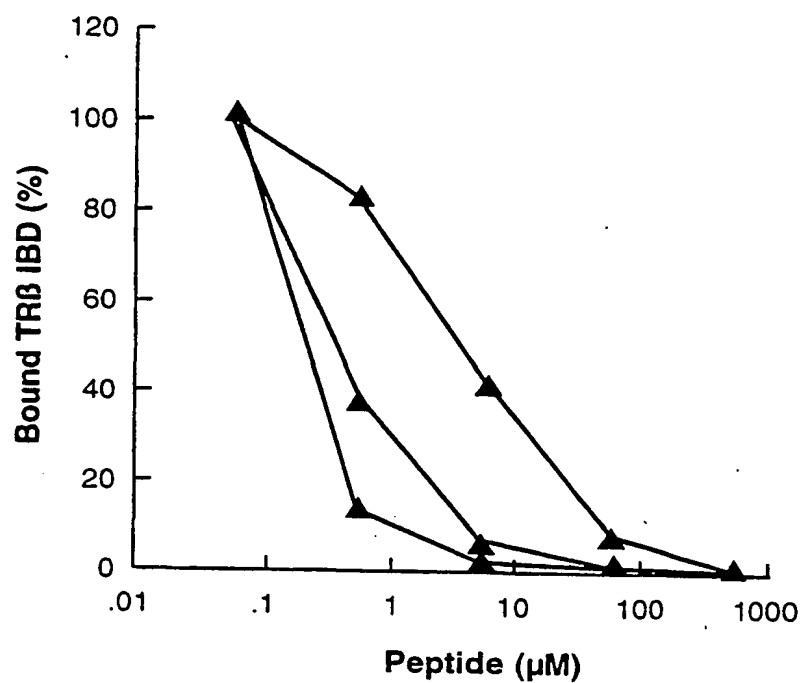
of SEQ ID No: 6

## FIGURE 10b



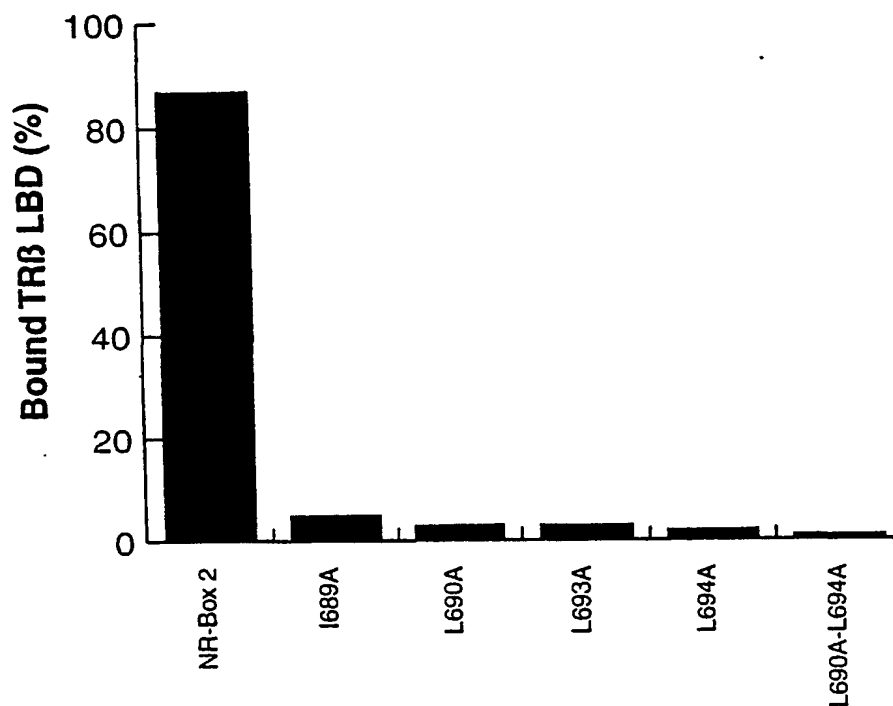


## FIGURE 10c



▲ Residues 8027 of SEQ ID No: 7	PKKKENA	LLRYLL	DKDDTKD
▲ Residues 11-27 of SEQ ID No: 6	TSLKEKHK	LLHRLL	QDSS
▲ SEQ ID No: 29	TSLKEKHK	LLRYLL	QDSS

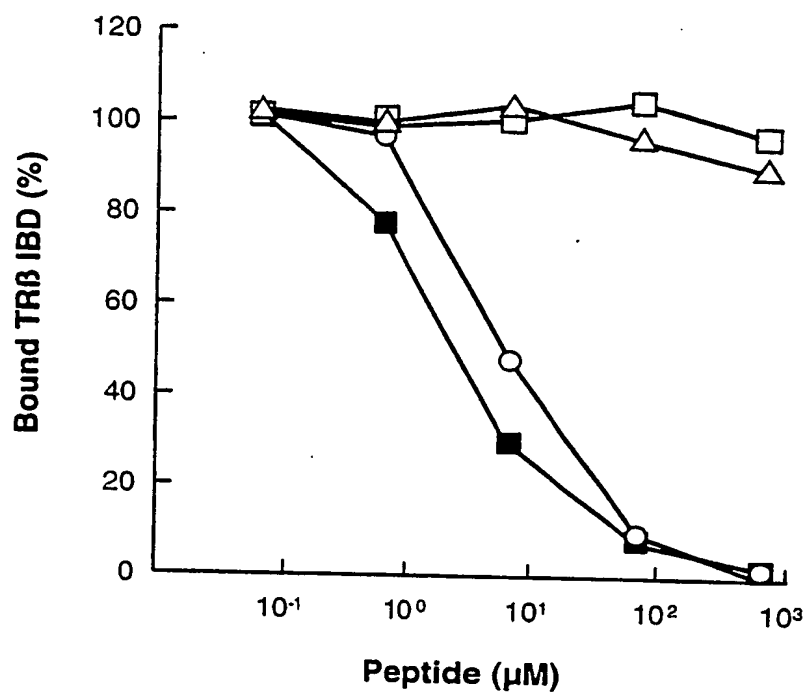
# FIGURE 11a



## NR-interaction domain:

NRb 1,2	ILHRLL
I689A	ALHRLL
L690A	IAHRLL
L693A	ILHRAL
L694A	ILHRLA
L690A/L694A	IAHRLA

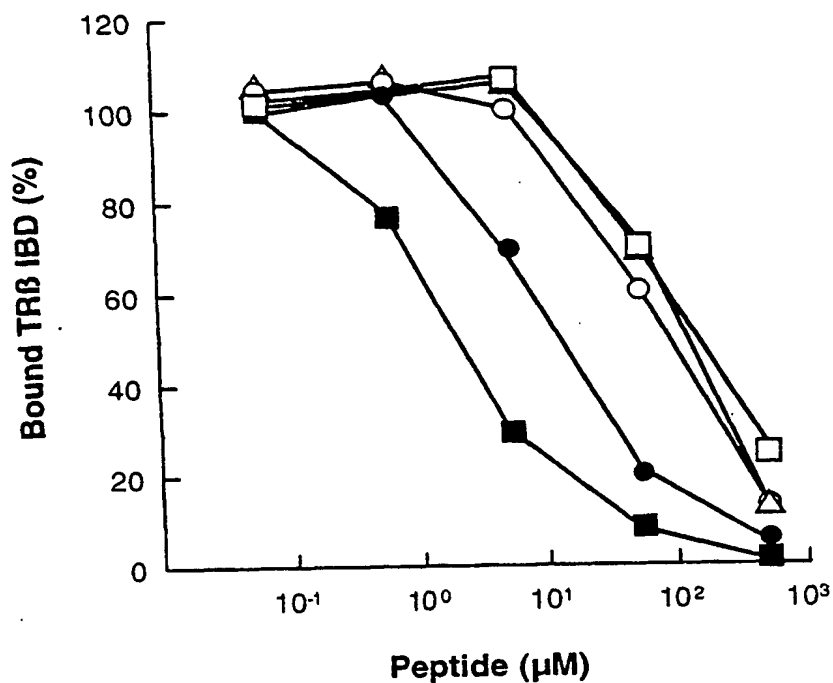
FIGURE 11b



Residues 12-24 SEQ ID No: 6

NR-Box 2 peptide: KHK ILLHRLL QDSS

- ILHRLL  
□ AAHRLL  
○ ILAALL  
△ ILHRAA

**FIGURE 11c**

Residues 12-24 SEQ ID No: 6

NR-Box 2 peptide: KHK **ILLHRLL** QDSS

- ILHRLL  
● FLHRLL  
□ IFHRLL  
○ ILHRFL  
△ ILHRLF

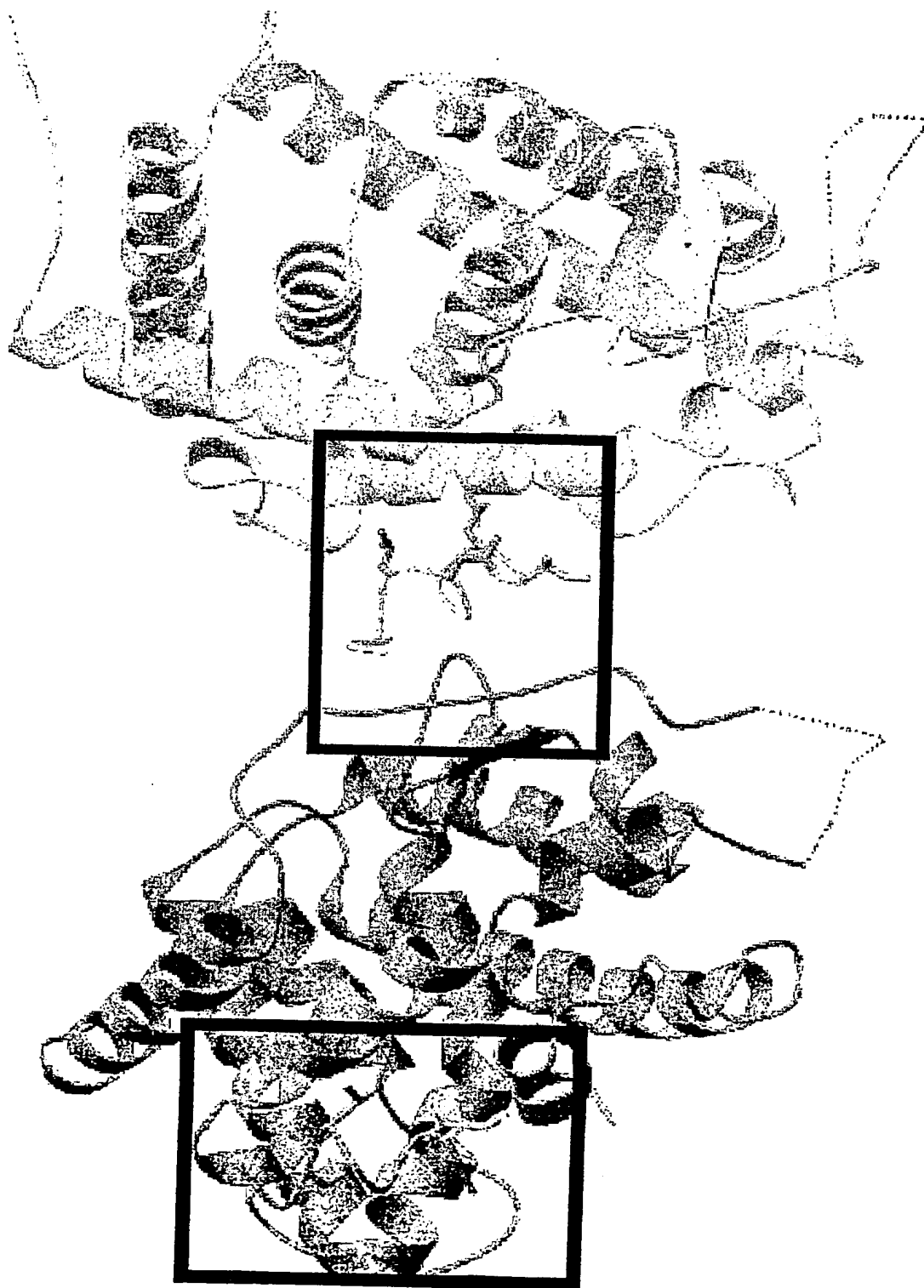
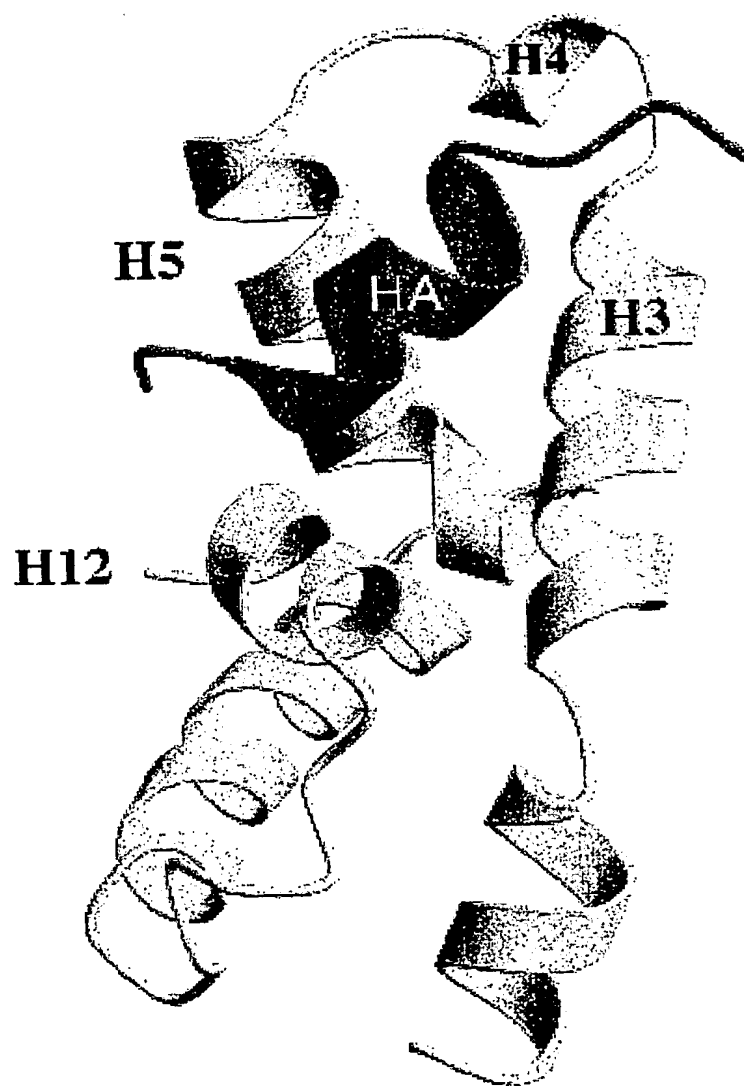
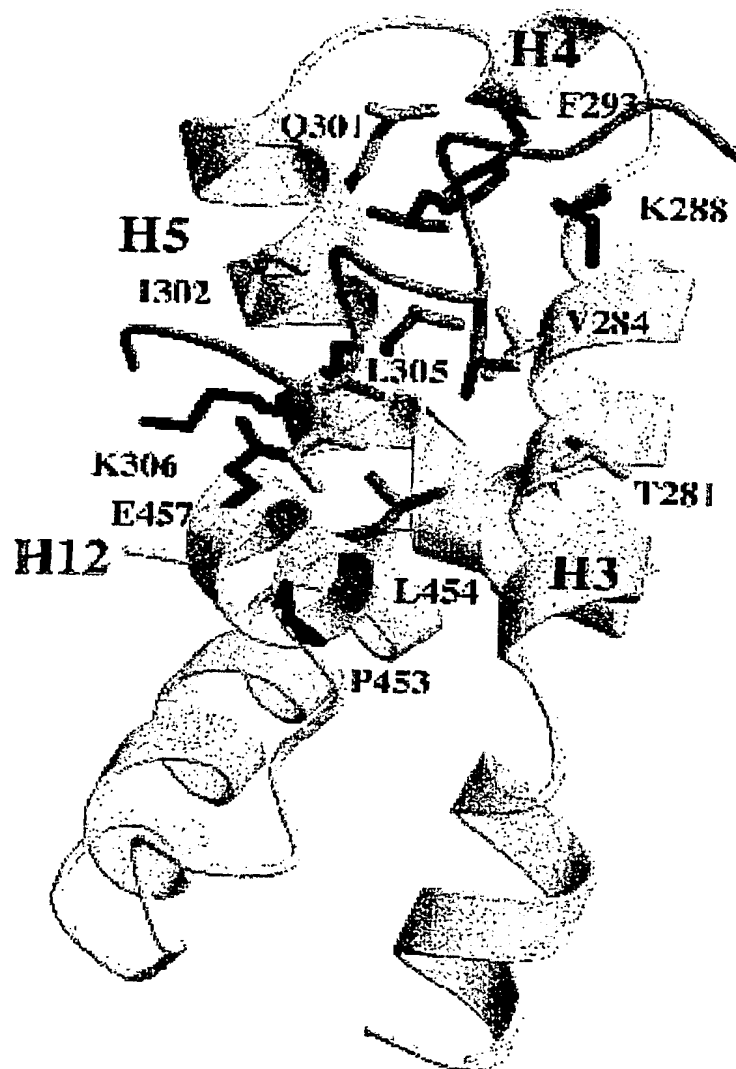


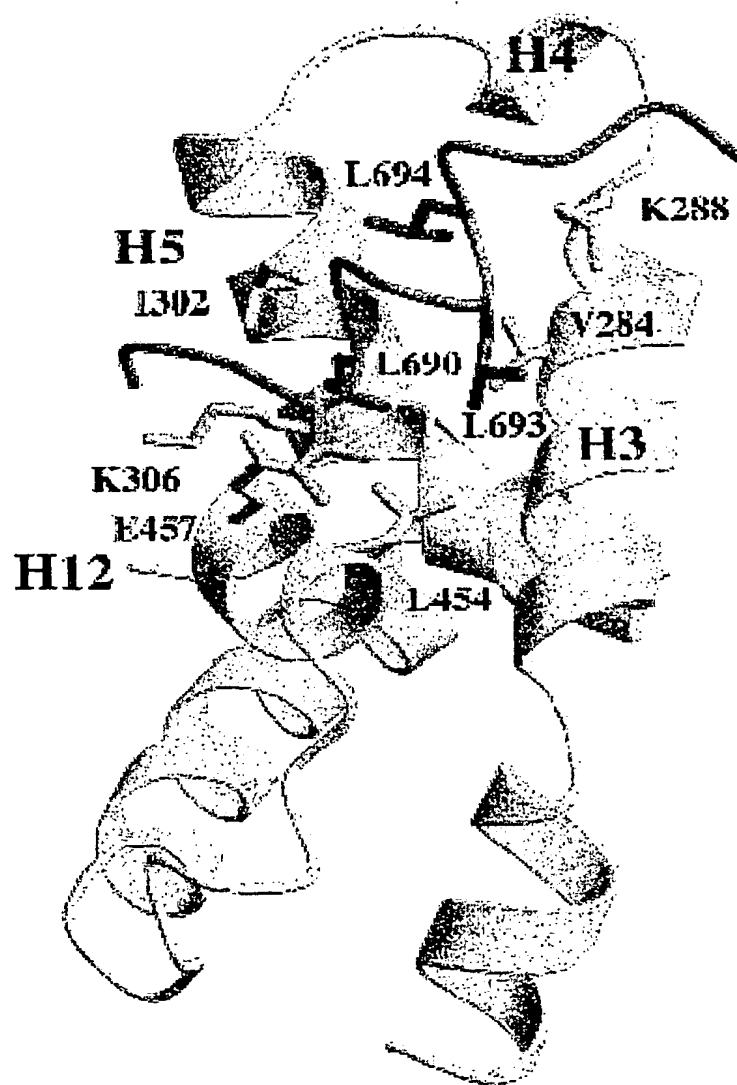
FIG. 12



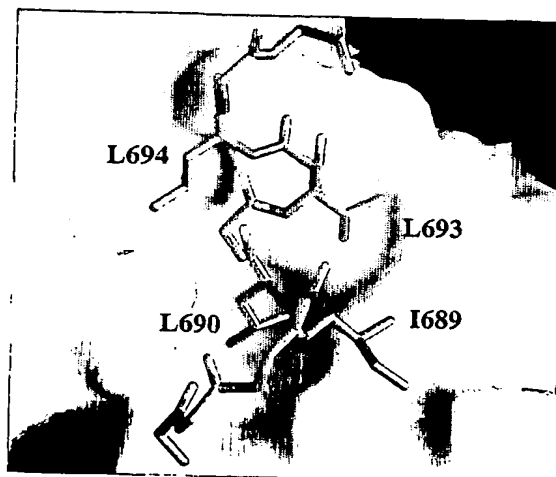
**FIG. 13**



**FIG. 14**

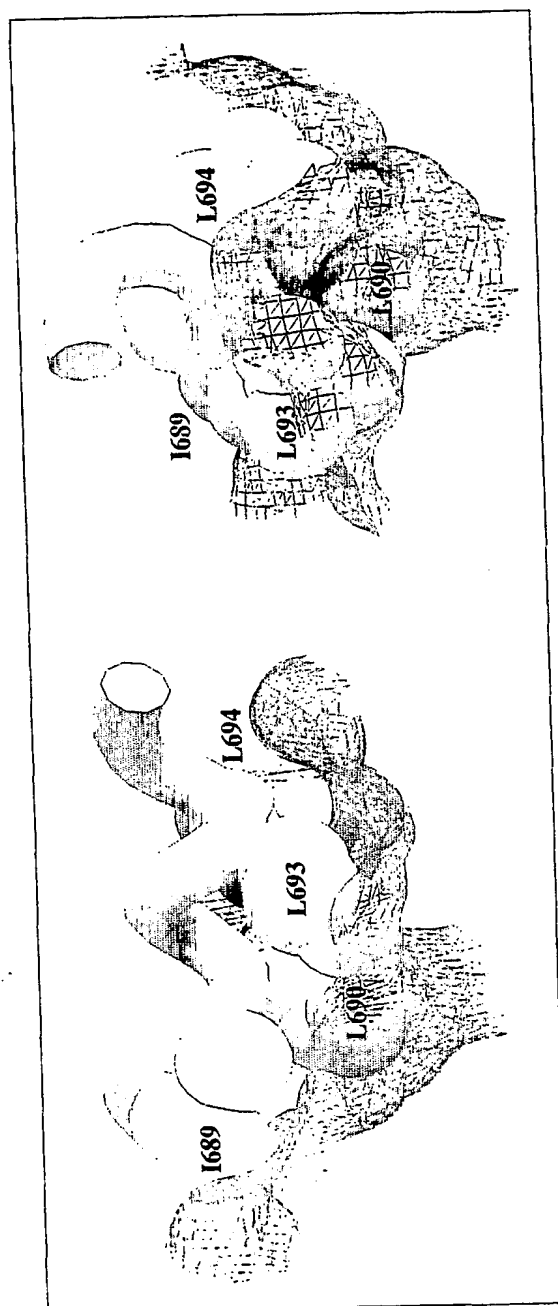
**FIG. 15**



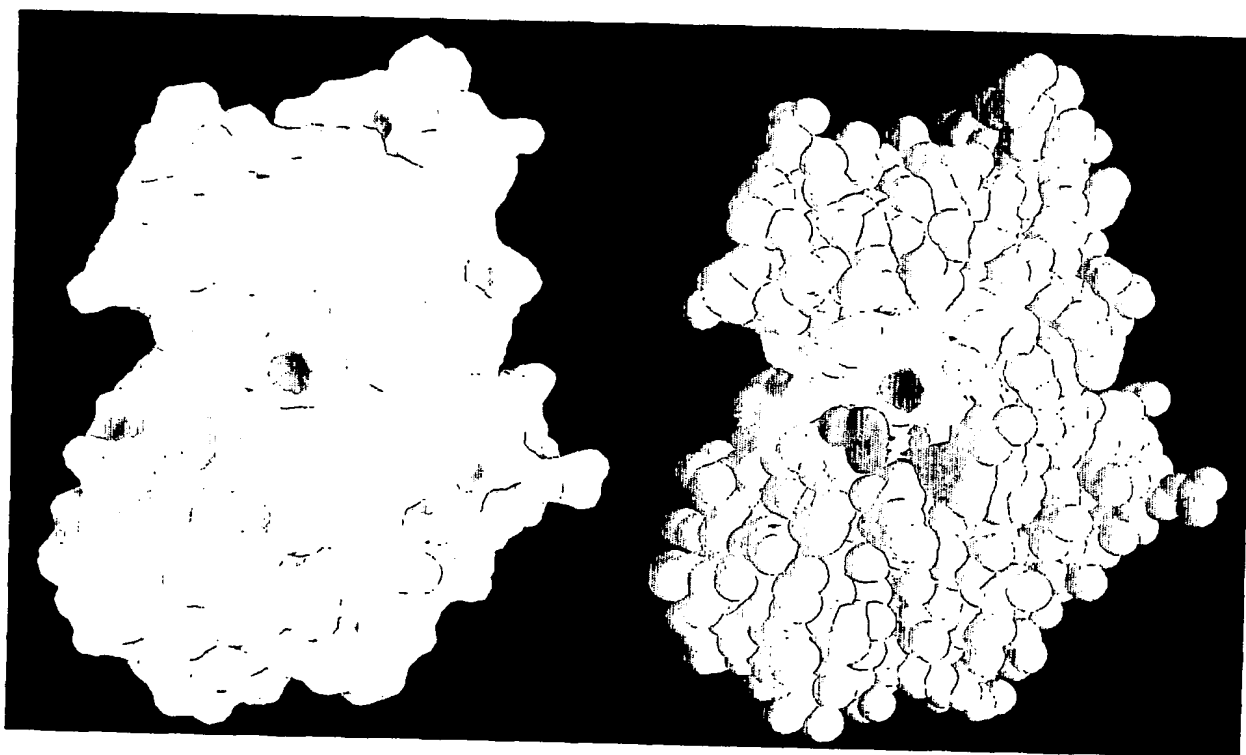


**FIG. 16**

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**FIG. 17**



**FIG. 18**

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309	hTRβ	301	hH3	287	hH3	288	hH3	293	hH4	305	hH5	306	hH6	309	hH6
277	hTRα	280	hH3	287	hH3	288	hH3	293	hH4	305	hH5	306	hH6	309	hH6
223	hRHRα	281	hH3	288	hH3	289	hH3	294	hH4	306	hH5	307	hH6	310	hH6
235	hRHRβ	282	hH3	290	hH3	291	hH3	295	hH4	307	hH5	308	hH6	311	hH6
273	hRHRγ	283	hH3	291	hH3	292	hH3	296	hH4	308	hH5	309	hH6	312	hH6
288	hRHRδ	284	hH3	292	hH3	293	hH3	297	hH4	309	hH5	310	hH6	313	hH6
235	hRHRε	285	hH3	293	hH3	294	hH3	298	hH4	310	hH5	311	hH6	314	hH6
351	hRHRζ	286	hH3	294	hH3	295	hH3	299	hH4	311	hH5	312	hH6	315	hH6
568	hRHRη	287	hH3	295	hH3	296	hH3	300	hH4	312	hH5	313	hH6	316	hH6
723	hRHRθ	288	hH3	296	hH3	297	hH3	301	hH4	313	hH5	314	hH6	317	hH6
774	hRHRι	289	hH3	297	hH3	298	hH3	302	hH4	314	hH5	315	hH6	318	hH6
242	hRHRκ	290	hH3	298	hH3	299	hH3	303	hH4	315	hH5	316	hH6	319	hH6

88Q	ID	NO:	31	b7Dg	450	F	P	P	L	F	L	E	V	F	F	E	D	461
88Q	ID	NO:	33	ETg	396	L	F	P	P	L	L	E	V	F	F	E	N	407
88Q	ID	NO:	35	b7AR	407	L	F	P	P	L	L	E	V	F	F	E	A	418
88Q	ID	NO:	37	b7Dg	446	L	F	P	P	L	L	E	V	F	F	E	A	457
88Q	ID	NO:	39	b7PARY	462	L	F	P	P	L	L	E	V	F	F	E	A	473
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## FIGURE 19

## 5 SEQUENCE LISTING

<110> Baxter, John D.  
Darimont, Beatrice  
Feng, Weijun  
10 Fletterick, Robert J.  
Kushner, Peter J.  
Wagner, Richard L.  
West, Brian L.  
15 Yamamoto, Keith R.

<120> METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR  
COACTIVATOR BINDING

<130> UCAL-253/01US

<140>

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<150> US 60/079,956

<151> 1998-03-30

<160> 51

<170> PatentIn Ver. 2.0

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1 5

<210> 2

<211> 6

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<400> 2

Ile Leu Xaa Xaa Leu Leu

1 5

<210> 3

<211> 5

<212> PRT

<213> Homo sapiens

<400> 3

Phe Xaa Xaa Leu Trp

1 5

<210> 4

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1 5

10 <210> 5  
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20 25 30  
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25 <210> 6  
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 20 <223> Leu --> Phe  
 <220>  
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 <222> (20)  
 25 <223> Leu --> Phe  
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 20 25 30  
 Thr Ala  
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 45 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Glu Ile Thr  
 20 25 30  
 50  
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 20 25 30  
 Ala Ser  
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5 <211> 34  
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 His Arg Leu Leu Gln Asp Ser Ser Ser Pro Val Asp Leu Ala Lys Leu  
                     20                    25                    30  
 15 Thr Ala  
  
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 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Glu Ile Thr  
 30                    20                    25                    30  
  
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                     20                    25                    30  
 45 Pro Ser  
  
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 55 Pro Gly Ser Thr His Gly Thr Ser Leu Lys Glu Lys His Lys Ile Leu  
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 His Arg Leu Leu Gln Asp Ser Ser Ser Pro Val Asp Leu Ala Lys Leu  
                     20                    25                    30  
 60 Thr Ala  
  
 65 <210> 13  
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5 <213> Homo sapiens

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 1 5 10 15

10 Leu Asp Lys Asp Asp Thr Lys Asp Ile Gly Leu Pro Ser Ile Thr  
 20 25 30

15 <210> 14  
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 Ala Glu Asn Gln Arg Gly Pro Leu Glu Ser Lys Gly His Lys Lys Leu  
 1 5 10 15

25 Leu Gln Leu Leu Thr Cys Ser Ser Glu Asp Arg Gly His Ser Ser Leu  
 20 25 30

Thr Asn

30 <210> 15  
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35 <400> 15  
 Thr Ser Asn Met His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu  
 1 5 10 15

40 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile  
 20 25 30

Thr Ala

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50 <400> 16  
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 1 5 10 15

55 Leu Leu Asp Arg Asp Asp Pro Ser Asp Val Leu Ala Lys Lys Leu Gln  
 20 25 30

60 <210> 17  
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65

5 <400> 17  
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     1                    5                    10                    15

10 Leu Gln Leu Leu Thr Cys Ser Ser Asp Asp Arg Gly His Ser Ser Leu  
                     20                    25                    30

Thr Asn

15 <210> 18  
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20 <400> 18  
 Thr Ser Asn Met His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu  
     1                    5                    10                    15

25 His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile  
                     20                    25                    30

Thr Ala

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<210> 19  
       <211> 32  
       <212> PRT  
       <213> Homo sapiens

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 Glu Gln Leu Ser Pro Lys Lys Lys Glu Asn Asn Ala Leu Leu Arg Tyr  
     1                    5                    10                    15

40 Leu Leu Asp Arg Asp Asp Pro Ser Asp Ala Leu Ser Lys Glu Leu Gln  
                     20                    25                    30

45

<210> 20  
       <211> 34  
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                     20                    25                    30

60 Thr Asn

65 <210> 21  
       <211> 34  
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&lt;400&gt; 21

Thr Ser Asn Val His Gly Ser Leu Leu Gln Glu Lys His Arg Ile Leu  
 1 5 10 15

10

His Lys Leu Leu Gln Asn Gly Asn Ser Pro Ala Glu Val Ala Lys Ile  
 20 25 30

Thr Ala

15

&lt;210&gt; 22

&lt;211&gt; 32

&lt;212&gt; PRT

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&lt;213&gt; Homo sapiens

&lt;400&gt; 22

Glu Gln Leu Ser Pro Lys Lys Lys Glu Asn Asn Ala Leu Leu Arg Tyr  
 1 5 10 15

25

Leu Leu Asp Arg Asp Asp Pro Ser Asp Ala Leu Ser Lys Glu Leu Gln  
 20 25 30

30

&lt;210&gt; 23

&lt;211&gt; 32

&lt;212&gt; PRT

35

&lt;213&gt; Homo sapiens

&lt;400&gt; 23

Ser Glu Gly Asp Ser Lys Tyr Ser Gln Thr Ser His Lys Leu Val Gln  
 1 5 10 15

40

Leu Leu Thr Thr Thr Ala Glu Gln Gln Leu Arg His Ala Asp Ile Asp  
 20 25 30

45

&lt;210&gt; 24

&lt;211&gt; 33

&lt;212&gt; PRT

50

&lt;213&gt; Homo sapiens

&lt;400&gt; 24

Thr Cys Pro Ser Ser His Ser Ser Leu Thr Glu Arg His Lys Ile Leu  
 1 5 10 15

55

His Arg Leu Leu Gln Glu Gly Ser Pro Ser Asp Ile Thr Thr Leu Ser  
 20 25 30

60

Val

65

&lt;210&gt; 25

&lt;211&gt; 34

&lt;212&gt; PRT

5 <213> Homo sapiens

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1 5 10 15

10 Arg Tyr Leu Leu Asp Lys Asp Glu Lys Asp Leu Arg Ser Thr Pro Asn  
20 25 30

Leu Cys

15

<210> 26

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20 <212> PRT

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25 <222> (2)

<223> negatively charged amino acid

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<223> hydrophobic amino acid

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35 <222> (25)

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<400> 26

Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Ser Xaa Xaa Xaa Xaa Lys Leu  
1 5 10 15

Xaa Gln Leu Leu Thr Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa  
20 25 30

45 Xaa Xaa

<210> 27

50 <211> 34

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<223> positively charged amino acid

<220>

65 <221> SITE

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 <221> SITE  
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 <223> negatively charged amino acid

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<220>  
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 <223> hydrophobic amino acid

15

<220>  
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 <222> (32)  
 <223> hydrophobic amino acid

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           1                                  5                                  10                                  15

25

His Xaa Leu Leu Gln Xaa Xaa Xaa Ser Pro Xaa Xaa Xaa Xaa Xaa Xaa  
                                   20                                  25                                  30

Xaa Xaa

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<220>  
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 <222> (24)  
 <223> negatively charged amino acid

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<220>  
 <221> SITE  
 <222> (33)  
 <223> hydrophobic amino acid

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<400> 28  
 Glu Xaa Xaa Xaa Xaa Lys Lys Lys Glu Xaa Xaa Xaa Xaa Xaa Leu Leu  
           1                                  5                                  10                                  15

55

Arg Tyr Leu Leu Asp Xaa Asp Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa Xaa  
                                   20                                  25                                  30

Xaa Xaa

60

<210> 29  
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65

5 <400> 29  
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     1                    5                    10                    15

10 Ser Ser

15 <210> 30  
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20 <220>  
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 <223> Thr --> Arg (T281R)

25 <220>  
 <221> MUTAGEN  
 <222> (8)  
 <223> Val --> Arg (V284R)

30 <220>  
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 <222> (9)  
 <223> Asp --> Ala (D285A)

35 <220>  
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 <222> (12)  
 <223> Lys --> Ala (K288A)

40 <220>  
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 <222> (22)  
 <223> Cys --> Arg (C298R)

45 <220>  
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 <223> Ile --> Arg (I302R)

50 <220>  
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 <223> Lys --> Ala (K306A)

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     1                    5                    10                    15

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                     20                    25                    30

60 Cys

65 <210> 31  
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 <213> Homo sapiens

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 <223> Glu --> Lys (E457K)

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25

<210> 32  
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35

Phe Ser Glu Leu Pro Cys Glu Asp Gln Ile Ile Leu Leu Lys Gly Cys  
                   20                  25                  30

Cys

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<210> 33  
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           1                  5                  10

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<210> 34  
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           1                  5                  10                  15

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Phe Thr Gly Leu Ser Ile Ala Asp Gln Ile Thr Leu Leu Lys Ala Ala  
                   20                  25                  30

Cys

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5 <210> 35  
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15 <210> 36  
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                     20                    25                    30

Trp

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40 <210> 38  
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Val

55 <210> 39  
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65 <210> 40



5 <211> 33  
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<400> 40  
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                     20                    25                    30  
 15 Ala

20 <210> 41  
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40 <220>  
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 <223> Val \_\_> Arg (V376R)

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                     20                    25                    30  
 Trp

55 <210> 43  
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 <213> Homo sapiens

60 <220>  
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 <223> Glu --> Lys (E542K)

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5            1                            5                            10

<210> 44

<211> 33

10 <212> PRT

<213> Homo sapiens

<400> 44

15 Gly Arg Gln Val Ile Ala Ala Val Lys Trp Ala Lys Ala Ile Pro Gly  
          1                            5                            10                            15

Phe Arg Asn Leu His Leu Asp Asp Gln Met Thr Leu Leu Gln Tyr Ser  
                          20                            25                            30

20 Trp

<210> 45

25 <211> 12

<212> PRT

<213> Homo sapiens

<400> 45

30 Glu Phe Pro Glu Met Leu Ala Glu Ile Ile Thr Asn  
          1                            5                            10

<210> 46

35 <211> 33

<212> PRT

<213> Homo sapiens

<400> 46

40 Glu Arg Gln Leu Leu Ser Val Val Lys Trp Ser Lys Ser Leu Pro Gly  
          1                            5                            10                            15

Phe Arg Asn Leu His Ile Asp Asp Gln Ile Thr Leu Ile Gln Tyr Ser  
                          20                            25                            30

45 Trp

50 <210> 47

<211> 12

<212> PRT

<213> Homo sapiens

55 <400> 47

Glu Phe Pro Glu Met Met Ser Glu Val Ile Ala Ala  
          1                            5                            10

60 <210> 48

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<212> PRT

<213> Homo sapiens

65 <400> 48

Gly Lys Gln Met Ile Gln Val Val Lys Trp Ala Lys Val Leu Pro Gly  
          1                            5                            10                            15

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Phe Lys Asn Leu Pro Leu Glu Asp Gln Ile Thr Leu Ile Gln Tyr Ser  
                     20                    25                    30

10

Trp

15

&lt;210&gt; 49

&lt;211&gt; 12

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

20

&lt;400&gt; 49

Glu Phe Pro Ala Met Leu Val Glu Ile Ile Ser Asp  
       1                    5                    10

25

&lt;210&gt; 50

&lt;211&gt; 33

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

30

&lt;400&gt; 50

Glu Arg Gln Leu Val His Val Val Lys Trp Ala Lys Ala Leu Pro Gly  
       1                    5                    10                    15

Phe Arg Asn Leu His Val Asp Asp Gln Met Ala Val Ile Gln Tyr Ser  
                     20                    25                    30

35

Trp

40

&lt;210&gt; 51

&lt;211&gt; 12

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

45

&lt;400&gt; 51

Asp Phe Pro Glu Met Met Ala Glu Ile Ile Ser Val  
       1                    5                    10

50

## INTERNATIONAL SEARCH REPORT

International application No.  
PCT/US99/06899

## A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) :G01N 33/50

US CL :435/7.1

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/7.1

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

Please See Extra Sheet.

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X ----- A	WAGNER et al. A structural role for hormone in the thyroid hormone receptor. Nature. 14 December 1995, Vol. 378, pages 690-697, especially page 690 and figure 1 and 2 and Table 1.	1 ----- 2-30

☐ Further documents are listed in the continuation of Box C.☐ See patent family annex.

* Special categories of cited documents:	*T* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
*A* document defining the general state of the art which is not considered to be of particular relevance	*X* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
*B* earlier document published on or after the international filing date	*Y* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
*L* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	*G* document member of the same patent family
*O* document referring to an oral disclosure, use, exhibition or other means	
*P* document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search

01 DECEMBER 1999

Date of mailing of the international search report

29 FEB 2000

Name and mailing address of the ISA/US  
Commissioner of Patents and Trademarks  
Box PCT  
Washington, D.C. 20231  
Facsimile No. (703) 305-3230

Authorized officer

MICHAEL PAK

Telephone No. (703) 308-1235

Form PCT/ISA/210 (second sheet)(July 1992)\*

## INTERNATIONAL SEARCH REPORT

International application No.  
PCT/US99/06899**Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)**

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:  
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claims Nos.:  
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
3. ☐ Claims Nos.:  
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

**Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)**

This International Searching Authority found multiple inventions in this international application, as follows:

Please See Extra Sheet.

1. ☒ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐  
☐

The additional search fees were accompanied by the applicant's protest.

No protest accompanied the payment of additional search fees.

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